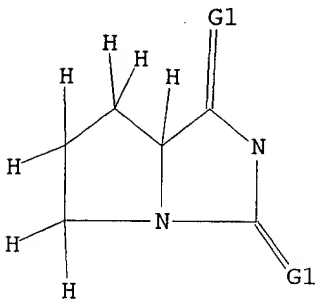
=> d
L1 HAS NO ANSWERS
L1 STR



G1 O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 09:24:43 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 89 TO ITERATE

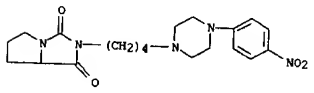
100.0% PROCESSED 89 ITERATIONS 11 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1214 TO 2346
PROJECTED ANSWERS: 22 TO 418

L2 11 SEA SSS SAM L1

=> d scan

L2 11 ANSWERS REGISTRY COPYRIGHT 2001 ACS
IN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-[4-(4-nitrophenyl)-1-piperazinyl]butyl]- (9CI)
MF C20 H27 N5 O4
CI COM



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

```
=> s l1 ful
FULL SEARCH INITIATED 09:24:59 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   1833 TO ITERATE

100.0% PROCESSED    1833 ITERATIONS                    224 ANSWERS
SEARCH TIME: 00.00.02

L3          224 SEA SSS FUL L1

=> s l3 and caplus/lc
      18958709 CAPLUS/LC
L4          215 L3 AND CAPLUS/LC

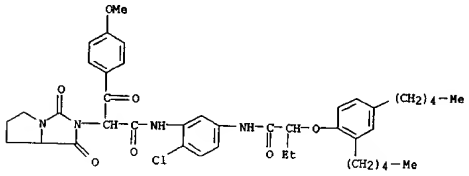
=> s l3 not l4
L5            9 L3 NOT L4

=> s l5 and caold/lc
       1435666 CAOLD/LC
L6            7 L5 AND CAOLD/LC

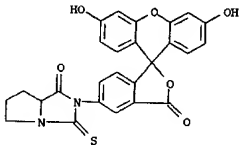
=> s l5 not l6
L7            2 L5 NOT L6

=> d 1-2
```

L7 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2001 ACS
RN 172018-43-8 REGISTRY
CN 1H-Pyrrolo[1,2-c]imidazole-2(3H)-acetamide, N-[2-chloro-5-[[2-(2,4-dipentylphenoxy)-1-oxobutyl]amino]phenyl]tetrahydro-.alpha.-(4-methoxybenzoyl)-1,3-dioxo- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C42 H51 Cl N4 O7
SR CAS Registry Services
LC STN Files: CHEMLIST



L7 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2001 ACS
RN 47758-46-3 REGISTRY
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)hexahydro-3-thioxo- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene], 1H-pyrrolo[1,2-c]imidazole deriv.
FS 3D CONCORD
MF C26 H18 N2 O6 S
CI COM



```
=> fil caold
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             145.09     145.24

FILE 'CAOLD' ENTERED AT 09:26:09 ON 04 SEP 2001
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2001 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1907-1966
FILE LAST UPDATED:  01 May 1997 (19970501/UP)

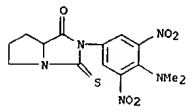
  This file contains CAS Registry Numbers for easy and accurate
  substance identification.  Title keywords, authors, patent
  assignees, and patent information, e.g., patent numbers, are
  now searchable from 1907-1966.  TIFF images of CA abstracts
  printed between 1907-1966 are available in the PAGE
  display formats.

  This file supports REG1stRY for direct browsing and searching of
  all substance data from the REGISTRY file.  Enter HELP FIRST for
  more information.

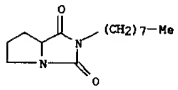
=> s l6
L8              5 L6

=> d 1-5 all hitstr
```

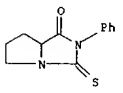
L8 ANSWER 1 OF 5 CAOLD COPYRIGHT 2001 ACS
AN CA60:13546f CAOLD
TI chromatographic sepn. of 4-dimethylamino-3,5-dinitrophenylthiohydantoins of amino acids
AU Neplyuev, V. M.; Chernukhina, L. A.; Serebryanyi, S. B.
IT 91347-65-8 91769-24-3 91909-02-3 92295-47-1 92297-37-5 92441-13-9 92441-16-2 92650-62-9 92654-49-4 93002-65-4 93571-26-7 93873-88-2
94162-87-5 95019-75-3 **96875-40-0** 97360-56-0 98840-59-6
IT **96875-40-0**
RN 96875-40-0 CAOLD
CN 1,2-Pyrrolidinedicarboximide, N-[4-(dimethylamino)-3,5-dinitrophenyl]-1-thio- (7CI) (CA INDEX NAME)



L8 ANSWER 2 OF 5 CAOLD COPYRIGHT 2001 ACS
AN CA60:2923b CAOLD
TI nucleophilic substitution reactions of fluoronitrobenzenes by methylimidazoles
AU Imbach, Jean L.; Jacquier, R.
IT 23309-18-4 23309-19-5 23309-20-8 23309-21-9 73225-15-7 88614-31-7 90946-21-7 91091-83-7 91211-64-2 91560-56-4 91695-74-8 92107-48-7 92289-71-9 92377-60-1 97237-78-0 **97359-06-3**
IT **97359-06-3**
RN 97359-06-3 CAOLD
CN 1,2-Pyrrolidinedicarboximide, N-octyl- (7CI) (CA INDEX NAME)

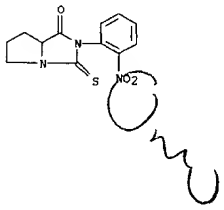


L8 ANSWER 3 OF 5 CAOLD COPYRIGHT 2001 ACS
AN CA52:983a CAOLD
TI detn. of amino acids as phenylthiohydantion derivs. - (I) micro synthesis of 3-phenyl-2-thiohydantoins from amino acids, (II) sepn. of 3-phenyl-2-thiohydantoins
AU Sjoquist, John
IT 2010-15-3 4332-95-0 4332-97-2 4333-19-1 4333-20-4 4333-21-5 4370-90-5 4399-40-0 4405-04-3 5066-94-4 5624-13-5 5624-27-1 5789-16-2 5789-21-9 5789-22-0 5789-24-2 5835-68-7 10567-81-4 **109070-15-7**
IT **109070-15-7**
RN 109070-15-7 CAOLD
CN 1,2-Pyrrolidinedicarboximide, hydroxy-N-phenyl-1-thio- (6CI) (CA INDEX NAME)

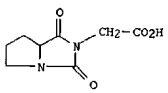


D1—OH

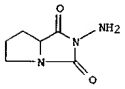
L8 ANSWER 4 OF 5 CAOLD COPYRIGHT 2001 ACS
AN CA51:17615c CAOLD
TI detn. of amino acids
AU Opienska-Blauth, Janina
TI infrared spectra of 3-phenyl-2-thiohydantoins of amino acids
AU Epp, Agnes
IT 2509-10-6 70172-78-0 99989-70-5 100115-26-2 100518-19-2 100610-91-1 101118-03-0 101351-90-0 101717-31-1 101722-31-0 101794-45-0 102026-63-1
102082-06-4 102082-08-6 102178-97-2 102665-95-2 102704-99-4 103395-94-4
108240-73-9 109068-49-7 109255-85-8 109509-57-1 109516-23-6 109654-58-2
109943-22-8 111066-92-3 111358-14-6 113510-88-6 **114911-12-5** 115231-34-0 118726-97-9
IT **114911-12-5**
RN 114911-12-5 CAOLD
CN 1,2-Pyrrolidinedicarboximide, N-(o-nitrophenyl)-1-thio- (6CI) (CA INDEX NAME)



L8 ANSWER 5 OF 5 CAOLD COPYRIGHT 2001 ACS
AN CA51:3572i CAOLD
TI peptides - (XIII) detn. of constitution of peptides (8) degradation of
methionine-, cystine-, serine-, proline-, tryptophan-, and histidine-peptides
AU Schloegl, K.; Wessely, F.; Woidich, H.
IT 103-46-8 2766-24-7 2766-31-6 2790-85-4 2899-67-4 3695-79-2 13515-86-1 13948-28-2 20210-01-9 98490-12-1 98636-54-5 99669-93-9
108748-69-2 108848-91-5 109337-23-7 109401-63-0 109498-12-6 109962-12-1 112627-09-5 114841-00-8 116956-12-8 **117122-03-9** 117627-76-6 **117885-95-7** 118802-51-0
IT **108748-69-2** **117122-03-9** **117885-95-7**
RN 108748-69-2 CAOLD
CN 1H-Pyrrolo[1,2-c]imidazole-2(3H)-acetic acid, tetrahydro-1,3-dioxo- (6CI)
(CA INDEX NAME)

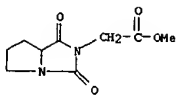


RN 117122-03-9 CAOLD
CN 1,2-Pyrrolidinedicarboximide, N-amino- (6CI) (CA INDEX NAME)



RN 117885-95-7 CAOLD
CN 1H-Pyrrolo[1,2-c]imidazole-2(3H)-acetic acid, tetrahydro-1,3-dioxo-, methyl ester (6CI) (CA INDEX NAME)

L8 ANSWER 5 OF 5 CAOLD COPYRIGHT 2001 ACS (Continued)



=> fil caplus
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	13.54	158.78

FILE 'CAPLUS' ENTERED AT 09:28:35 ON 04 SEP 2001
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1947 - 4 Sep 2001 VOL 135 ISS 11
FILE LAST UPDATED: 3 Sep 2001 (20010903/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

CAplus now provides online access to patents and literature covered in CA from 1947 to the present. On April 22, 2001, bibliographic information and abstracts were added for over 2.2 million references published in CA from 1947 to 1966.

The CA Lexicon is now available in the Controlled Term (/CT) field. Enter HELP LEXICON for full details.

*** YOU HAVE NEW MAIL ***

=> s l3

L9 208 L3

=> fil reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.33	159.11

FILE 'REGISTRY' ENTERED AT 09:28:50 ON 04 SEP 2001
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

STRUCTURE FILE UPDATES: 3 SEP 2001 HIGHEST RN 354528-22-6
DICTIONARY FILE UPDATES: 3 SEP 2001 HIGHEST RN 354528-22-6

TSCA INFORMATION NOW CURRENT THROUGH January 11, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

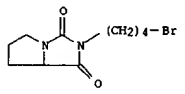
Structure search limits have been increased. See HELP SLIMIT for details.

```
=> s l3 and ref.caplus<5
      18380171 REF.CAPLUS<5
L10         204 L3 AND REF.CAPLUS<5

=> s l3 not l10
L11          20 L3 NOT L10

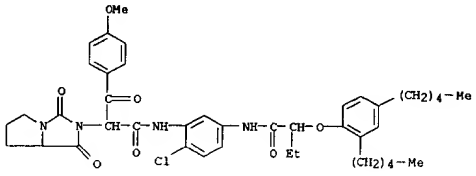
=> d 1-20
```

L11 ANSWER 1 OF 20 REGISTRY COPYRIGHT 2001 ACS
RN 181948-88-9 REGISTRY
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(4-bromobutyl)tetrahydro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C10 H15 Br N2 O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXLIT



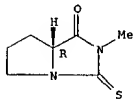
6 REFERENCES IN FILE CA (1967 TO DATE)
6 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L11 ANSWER 2 OF 20 REGISTRY COPYRIGHT 2001 ACS
RN 172018-43-8 REGISTRY
CN 1H-Pyrrolo[1,2-c]imidazole-2(3H)-acetamide, N-[2-chloro-5-[[2-(2,4-dipentylphenoxy)-1-oxobutyl]amino]phenyl]tetrahydro-.alpha.-(4-methoxybenzoyl)-1,3-dioxo- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C42 H51 Cl N4 O7
SR CAS Registry Services
LC STN Files: CHEMLIST



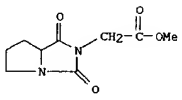
L11 ANSWER 3 OF 20 REGISTRY COPYRIGHT 2001 ACS
RN 145552-40-5 REGISTRY
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo-, (7aR)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo-, (R)-
FS STEREOSEARCH
MF C7 H10 N2 O S
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.



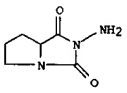
9 REFERENCES IN FILE CA (1967 TO DATE)
9 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L11 ANSWER 4 OF 20 REGISTRY COPYRIGHT 2001 ACS
RN 117885-95-7 REGISTRY
CN 1H-Pyrrolo[1,2-c]imidazole-2(3H)-acetic acid, tetrahydro-1,3-dioxo-, methyl ester (6CI) (CA INDEX NAME)
FS 3D CONCORD
MF C9 H12 N2 O4
SR CAOLD
LC STN Files: BEILSTEIN*, CAOLD
(*File contains numerically searchable property data)



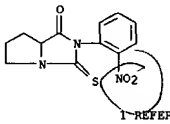
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L11 ANSWER 5 OF 20 REGISTRY COPYRIGHT 2001 ACS
RN 117122-03-9 REGISTRY
CN 1,2-Pyrrolidinedicarboximide, N-amino- (6CI) (CA INDEX NAME)
FS 3D CONCORD
MF C6 H9 N3 O2
SR CAOLD
LC STN Files: BEILSTEIN*, CAOLD
(*File contains numerically searchable property data)



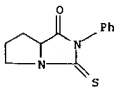
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L11 ANSWER 6 OF 20 REGISTRY COPYRIGHT 2001 ACS
RN 114911-12-5 REGISTRY
CN 1,2-Pyrrolidinedicarboximide, N-(o-nitrophenyl)-1-thio- (6CI) (CA INDEX
NAME)
FS 3D CONCORD
MF C12 H11 N3 O3 S
SR CAOLD
LC STN Files: BEILSTEIN*, CAOLD
(*File contains numerically searchable property data)



1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

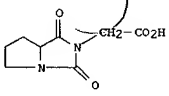
L11 ANSWER 7 OF 20 REGISTRY COPYRIGHT 2001 ACS
RN 109070-15-7 REGISTRY
CN 1,2-Pyrrolidinedicarboximide, hydroxy-N-phenyl-1-thio- (6CI) (CA INDEX
NAME)
MF C12 H12 N2 O2 S
CI IDS
SR CAOLD
LC STN Files: CAOLD



D1-OH

2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

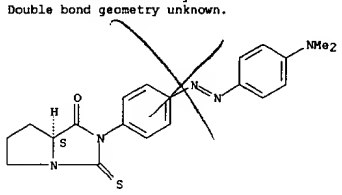
L11 ANSWER 8 OF 20 REGISTRY COPYRIGHT 2001 ACS
RN 108748-69-2 REGISTRY
CN 1H-Pyrrolo[1,2-c]imidazole-2(3H)-acetic acid, tetrahydro-1,3-dioxo- (6CI)
(CA INDEX NAME)
FS 3D CONCORD
MF C8 H10 N2 O4
SR CAOLD
LC STN Files: BEILSTEIN*, CAOLD
(*File contains numerically searchable property data)



1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

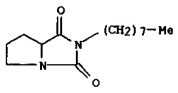
L11 ANSWER 9 OF 20 REGISTRY COPYRIGHT 2001 ACS
RN 103697-53-6 REGISTRY
CN 1H-Pyrrolo[1,2-c]imidazol-1-one,
2-[4-[[4-(dimethylamino)phenyl]azo]phenyl
]hexahydro-3-thioxo-, (S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C20 H21 N5 O S
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry unknown.



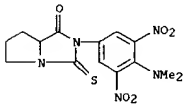
5 REFERENCES IN FILE CA (1967 TO DATE)
5 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L11 ANSWER 10 OF 20 REGISTRY COPYRIGHT 2001 ACS
RN 97359-06-3 REGISTRY
CN 1,2-Pyrrolidinedicarboximide, N-octyl- (7CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H24 N2 O2
SR CAOLD
LC STN Files: BEILSTEIN*, CAOLD
(*File contains numerically searchable property data)



1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

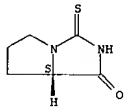
L11 ANSWER 11 OF 20 REGISTRY COPYRIGHT 2001 ACS
RN 96875-40-0 REGISTRY
CN 1,2-Pyrrolidinedicarboximide,
N-[4-(dimethylamino)-3,5-dinitrophenyl]-1-
thio- (7CI) (CA INDEX NAME)
MF C14 H15 N5 O5 S
LC STN Files: BEILSTEIN*, CAOLD
(*File contains numerically searchable property data)



1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

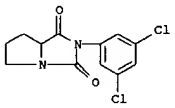
L11 ANSWER 12 OF 20 REGISTRY COPYRIGHT 2001 ACS
RN 61160-12-1 REGISTRY
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-3-thioxo-, (7aS)- (9CI)
(CA
INDEX NAME)
OTHER CA INDEX NAMES:
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-3-thioxo-, (S)-
FS STEREOSEARCH
MF C6 H8 N2 O S
LC STN Files: BEILSTEIN*, CA, CAPLUS, MEDLINE, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry.



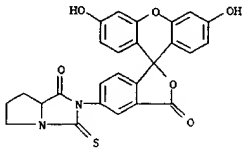
9 REFERENCES IN FILE CA (1967 TO DATE)
9 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L11 ANSWER 13 OF 20 REGISTRY COPYRIGHT 2001 ACS
RN 60725-79-3 REGISTRY
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(3,5-dichlorophenyl)tetrahydro- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H10 Cl2 N2 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



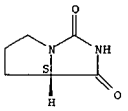
5 REFERENCES IN FILE CA (1967 TO DATE)
5 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L11 ANSWER 14 OF 20 REGISTRY COPYRIGHT 2001 ACS
RN 47758-46-3 REGISTRY
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)hexahydro-3-thioxo- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene], 1H-pyrrolo[1,2-c]imidazole deriv.
FS 3D CONCORD
MF C26 H18 N2 O6 S
CI COM



L11 ANSWER 15 OF 20 REGISTRY COPYRIGHT 2001 ACS
RN 40856-87-9 REGISTRY
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-, (7aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-, (S)-
FS STEREOSEARCH
MF C6 H8 N2 O2
LC STN Files: BEILSTEIN*, CA, CANCERLIT, CAPLUS, MEDLINE, TOXLINE, TOXLIT
(*File contains numerically searchable property data)

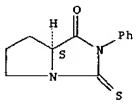
Absolute stereochemistry.



14 REFERENCES IN FILE CA (1967 TO DATE)
14 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L11 ANSWER 16 OF 20 REGISTRY COPYRIGHT 2001 ACS
RN 29635-99-2 REGISTRY
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,2-Pyrrolidinedicarboximide, N-phenyl-1-thio-, L- (8CI)
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (S)-
OTHER NAMES:
CN L-Proline phenylthiohydantoin
CN Phenylthiohydantoin L-proline
CN Proline phenylthiohydantoin
CN PTH-Proline
FS STEREOSEARCH
MF C12 H12 N2 O S
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS, CSCHEM, MSDS-OHS
(*File contains numerically searchable property data)

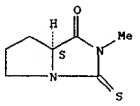
Absolute stereochemistry.



61 REFERENCES IN FILE CA (1967 TO DATE)
61 REFERENCES IN FILE CAPLUS (1967 TO DATE)

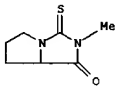
L11 ANSWER 17 OF 20 REGISTRY COPYRIGHT 2001 ACS
RN 28868-23-7 REGISTRY
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,2-Pyrrolidinedicarboximide, N-methyl-1-thio-, L- (8CI)
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo-, (S)-
FS STEREOSEARCH
MF C7 H10 N2 O S
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)

Absolute stereochemistry.



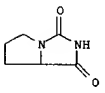
13 REFERENCES IN FILE CA (1967 TO DATE)
13 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L11 ANSWER 18 OF 20 REGISTRY COPYRIGHT 2001 ACS
RN 22712-58-9 REGISTRY
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,2-Pyrrolidinedicarboximide, N-methyl-1-thio- (6CI, 7CI, 8CI)
OTHER NAMES:
CN Proline, 3-methyl-2-thiohydantoin
FS 3D CONCORD
DR 1968-34-9
MF C7 H10 N2 O S
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CHEMCATS, CSCHEM, TOXLIT
(*File contains numerically searchable property data)



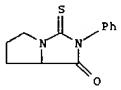
15 REFERENCES IN FILE CA (1967 TO DATE)
15 REFERENCES IN FILE CAPLUS (1967 TO DATE)
3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L11 ANSWER 19 OF 20 REGISTRY COPYRIGHT 2001 ACS
RN 5768-79-6 REGISTRY
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,2-Pyrrolidinedicarboximide (7CI, 8CI)
OTHER NAMES:
CN 1,5-Trimethylenehydantoin
CN Proline hydantoin
FS 3D CONCORD
MF C6 H8 N2 O2
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMLIST, TOXLIT,
USPATFULL
(*File contains numerically searchable property data)



17 REFERENCES IN FILE CA (1967 TO DATE)
17 REFERENCES IN FILE CAPLUS (1967 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L11 ANSWER 20 OF 20 REGISTRY COPYRIGHT 2001 ACS
RN 4333-21-5 REGISTRY
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,2-Pyrrolidinedicarboximide, N-phenyl-1-thio- (6CI, 7CI, 8CI)
OTHER NAMES:
CN Phenylthiohydantoin DL-proline
CN Proline phenylthiohydantoin
FS 3D CONCORD
DR 31364-82-6
MF C12 H12 N2 O S
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CHEMCATS, CHEMLIST, CSCHEM,
TOXLIT
(*File contains numerically searchable property data)
Other Sources: EINECS**
(**Enter CHEMLIST File for up-to-date regulatory information)



25 REFERENCES IN FILE CA (1967 TO DATE)
25 REFERENCES IN FILE CAPLUS (1967 TO DATE)
17 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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=> fil caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                              31.55     190.66

FILE 'CAPLUS' ENTERED AT 09:31:34 ON 04 SEP 2001
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2001 AMERICAN CHEMICAL SOCIETY (ACS)
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FILE COVERS 1947 - 4 Sep 2001  VOL 135 ISS 11
FILE LAST UPDATED: 3 Sep 2001  (20010903/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.

  This file supports REGistRY for direct browsing and searching of
  all substance data from the REGISTRY file.  Enter HELP FIRST for
  more information.

CAplus now provides online access to patents and literature covered
in CA from 1947 to the present.  On April 22, 2001, bibliographic
information and abstracts were added for over 2.2 million references
published in CA from 1947 to 1966.

The CA Lexicon is now available in the Controlled Term (/CT) field.
Enter HELP LEXICON for full details.
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*** YOU HAVE NEW MAIL ***

=> d his

     (FILE 'HOME' ENTERED AT 09:23:58 ON 04 SEP 2001)

     FILE 'REGISTRY' ENTERED AT 09:24:00 ON 04 SEP 2001
L1             STRUCTURE UPLOADED
L2              11 S L1
L3             224 S L1 FUL
L4             215 S L3 AND CAPLUS/LC
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L5             9 S L3 NOT L4
L6             7 S L5 AND CAOLD/LC
L7             2 S L5 NOT L6

     FILE 'CAOLD' ENTERED AT 09:26:09 ON 04 SEP 2001
L8             5 S L6

     FILE 'CAPLUS' ENTERED AT 09:28:35 ON 04 SEP 2001
L9           208 S L3

     FILE 'REGISTRY' ENTERED AT 09:28:50 ON 04 SEP 2001
L10          204 S L3 AND REF.CAPLUS<5
L11           20 S L3 NOT L10

     FILE 'CAPLUS' ENTERED AT 09:31:34 ON 04 SEP 2001

=> d sort l9 occ 1-208
'SORT' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

The following are valid formats:

ABS --------- GI and AB
ALL --------- BIB, AB, IND, RE
APPS -------- AI, PRAI
BIB --------- AN, plus Bibliographic Data and PI table (default)
CAN --------- List of CA abstract numbers without answer numbers
CBIB -------- AN, plus Compressed Bibliographic Data
DALL -------- ALL, delimited (end of each field identified)
DMAX -------- MAX, delimited for post-processing
FAM --------- AN, PI and PRAI in table, plus Patent Family data
FBIB -------- AN, BIB, plus Patent FAM
IND --------- Indexing data
IPC --------- International Patent Classifications
MAX --------- ALL, plus Patent FAM, RE
PATS -------- PI, SO
SAM --------- CC, SX, TI, ST, IT
SCAN -------- CC, SX, TI, ST, IT (random display, no answer numbers;
              SCAN must be entered on the same line as the DISPLAY,
              e.g., D SCAN or DISPLAY SCAN)
STD --------- BIB, IPC, and NCL

IABS -------- ABS, indented with text labels
IALL -------- ALL, indented with text labels
IBIB -------- BIB, indented with text labels
IMAX -------- MAX, indented with text labels
ISTD -------- STD, indented with text labels

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
```

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SIBIB ------- IBIB, no citations

HIT --------- Fields containing hit terms
HITIND ------ IC, ICA, ICI, NCL, CC and index field (ST and IT)
              containing hit terms
HITRN ------- HIT RN and its text modification
HITSTR ------ HIT RN, its text modification, its CA index name, and
              its structure diagram
FHITSTR ----- First HIT RN, its text modification, its CA index name, and
              its structure diagram
KWIC -------- Hit term plus 20 words on either side
OCC --------- Number of occurrence of hit term and field in which it occurs

To display a particular field or fields, enter the display field
codes.  For a list of the display field codes, enter HELP DFIELDS at
an arrow prompt (=>).  Examples of formats include: TI; TI,AU; BIB,ST;
TI,IND; TI,SO.  You may specify the format fields in any order and the
information will be displayed in the same order as the format
specification.

All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR,
FHITSTR, KWIC, and OCC) may be used with DISPLAY ACC to view a
specified Accession Number.
ENTER DISPLAY FORMAT (BIB):end

=> sort l9 occ 1-208
PROCESSING COMPLETED FOR L9
L12          208 SORT L9 1-208 OCC

=> d ibib abs hitstr 1-20
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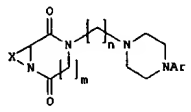
L12 ANSWER 1 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1996:422371 CAPLUS
DOCUMENT NUMBER: 125:86677
TITLE: New arylpiperazine derivatives useful as 5-HT1A ligands.
INVENTOR(S): Lopez Rodriquez, Maria Luz; Rosado Samitier, Maria Luisa; Benahu Salama, Bellinda; Fernandez Velando, Esther; Morcillo Ortega, Maria Jose
PATENT ASSIGNEE(S): Universidad Complutense De Madrid, Spain
SOURCE: PCT Int. Appl., 20 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Spanish
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9606846	A1	19960307	WO 1995-ES94	19950728
W: AU, CA, JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
ES 2082727	A1	19960316	ES 1994-1895	19940901
ES 2082727	B1	19961016		
AU 9530792	A1	19960322	AU 1995-30792	19950728
ES 2095811	A1	19970216	ES 1995-1534	19950728
ES 2095811	B1	19970801		

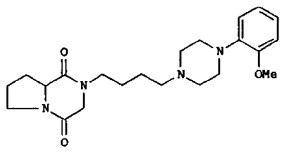
PRIORITY APPLN. INFO.: ES 1994-1895 19940901
ES 1995-1534 19950728
WO 1995-ES94 19950728

OTHER SOURCE(S): MARPAT 125:86677
GI

L12 ANSWER 1 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



I



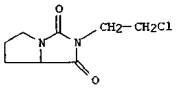
II

AB The invention relates to new compds. of formula I [X = (CH2)3 or (CH2)4; m = 0 or 1; n = 1, 2, 3, or 4; Ar = 1-naphthyl, 7-benzofuranyl, 2,3-dihydro-1,4-benzodioxan-5-yl, 3,4-dihydro-2H-1,5-benzodioxepin-6-yl, Ph, or Ph substituted by alkyl, halo, CF3, NO2, cyano, alkoxy, amino, alkylcarbamoyl, alkylsulfonamido, or alkoxycarbonyl]. The invention also relates to various alternative methods for the prepn. of I. The compds. show an affinity for the serotoninergic receptor 5-HT1A, which indicates their therapeutic utility in the treatment of CNS disorders such as anxiety and depression. For example, 1,4-dioxoperhydropyrrolo[1,2-a]pyrazine underwent N-alkylation with NaH and Br(CH2)4Cl in DMF at 60-110.degree.. This was followed by N-alkylation of 1-(o-methoxyphenyl)piperazine, using the product of the previous step and Et3N in refluxing MeCN, to give title compd. II. In an assay for displacement of [3H]-8-OH-DPAT from rat cerebral 5-HT1A receptors in vitro, selected I had Ki ranging from 1.2 nM to 341 nM.

IT **178482-71-8P**, 2-(2-Chloroethyl)-1,3-dioxoperhydropyrrolo[1,2-c]imidazole
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(intermediate; prepn. of arylpiperazine derivs. as 5-HT1A ligands)

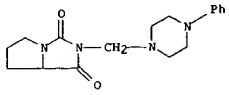
RN 178482-71-8 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(2-chloroethyl)tetrahydro-

L12 ANSWER 1 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
(9CI) (CA INDEX NAME)



IT **178481-97-5P 178481-98-6P 178481-99-7P**
178482-00-3P 178482-01-4P 178482-02-5P
178482-03-6P 178482-11-6P 178482-12-7P
178482-13-8P 178482-14-9P 178482-15-0P
178482-16-1P 178482-27-4P 178482-28-5P
178482-29-6P 178482-30-9P 178482-31-0P
178482-32-1P 178482-33-2P 178482-34-3P
178482-35-4P 178482-36-5P 178482-54-7P
178482-55-8P 178482-56-9P 178482-57-0P
178482-58-1P 178482-59-2P 178482-60-5P
178482-61-6P 178482-62-7P 178482-63-8P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of arylpiperazine derivs. as 5-HT1A ligands)

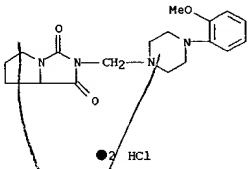
RN 178481-97-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[(4-phenyl-1-piperazinyl)methyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

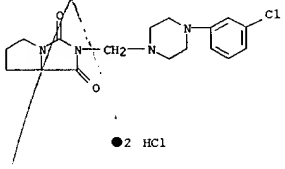
RN 178481-98-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]-, dihydrochloride (9CI) (CA INDEX NAME)

L12 ANSWER 1 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



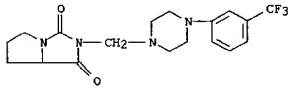
●2 HCl

RN 178481-99-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[[4-(3-chlorophenyl)-1-piperazinyl]methyl]tetrahydro-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

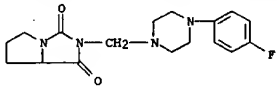
RN 178482-00-3 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]methyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

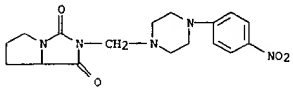
RN 178482-01-4 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[[4-(4-fluorophenyl)-1-piperazinyl]methyl]tetrahydro-, dihydrochloride (9CI) (CA INDEX NAME)

L12 ANSWER 1 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



●2 HCl

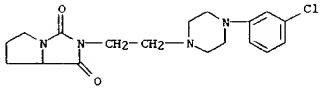
RN 178482-02-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[[4-(4-nitrophenyl)-1-piperazinyl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

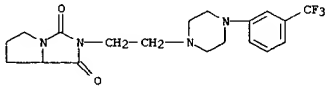
RN 178482-03-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[[4-(1-naphthalenyl)-1-piperazinyl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

L12 ANSWER 1 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[2-[4-(3-chlorophenyl)-1-piperazinyl]ethyl]tetrahydro-, dihydrochloride (9CI) (CA INDEX NAME)



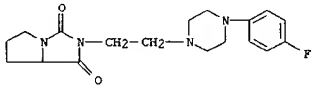
●2 HCl

RN 178482-14-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[2-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]ethyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

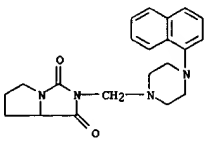
RN 178482-15-0 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[2-[4-(4-fluorophenyl)-1-piperazinyl]ethyl]tetrahydro-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

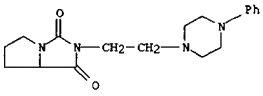
RN 178482-16-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[2-[4-(4-nitrophenyl)-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)

L12 ANSWER 1 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

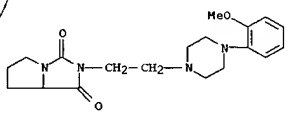


● HCl

RN 178482-11-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[2-(4-phenyl-1-piperazinyl)ethyl]- (9CI) (CA INDEX NAME)



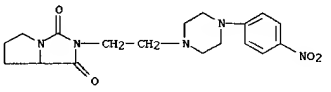
RN 178482-12-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[2-[4-(2-methoxyphenyl)-1-piperazinyl]ethyl]-, dihydrochloride (9CI) (CA INDEX NAME)



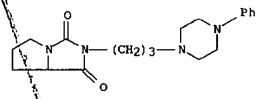
●2 HCl

RN 178482-13-8 CAPLUS

L12 ANSWER 1 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

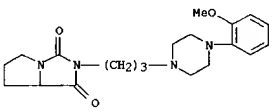


RN 178482-27-4 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[3-(4-phenyl-1-piperazinyl)propyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

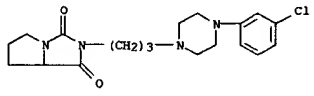
RN 178482-28-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[3-[4-(2-methoxyphenyl)-1-piperazinyl]propyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

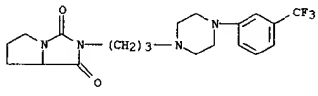
RN 178482-29-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[3-[4-(3-chlorophenyl)-1-piperazinyl]propyl]tetrahydro-, dihydrochloride (9CI) (CA INDEX NAME)

L12 ANSWER 1 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



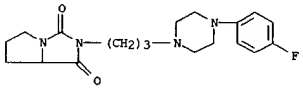
●2 HCl

RN 178482-30-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[3-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]propyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

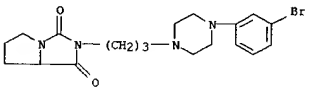
RN 178482-31-0 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[3-[4-(4-fluorophenyl)-1-piperazinyl]propyl]tetrahydro-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

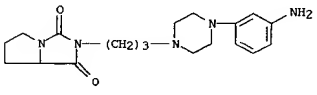
RN 178482-32-1 CAPLUS

L12 ANSWER 1 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



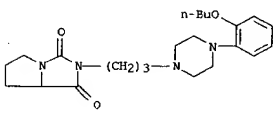
●2 HCl

RN 178482-35-4 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[3-[4-(3-aminophenyl)-1-piperazinyl]propyl]tetrahydro-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

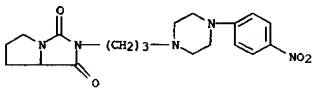
RN 178482-36-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[3-[4-(2-butoxyphenyl)-1-piperazinyl]propyl]tetrahydro-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

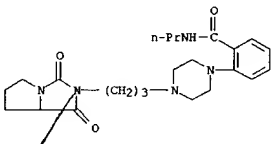
RN 178482-54-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-(4-phenyl-1-piperazinyl)butyl]-, dihydrochloride (9CI) (CA INDEX NAME)

L12 ANSWER 1 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



● HCl

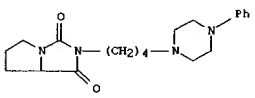
RN 178482-33-2 CAPLUS
CN Benzamide, N-propyl-2-[4-[3-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)propyl]-1-piperazinyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

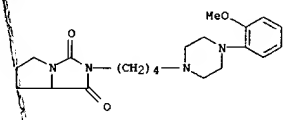
RN 178482-34-3 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[3-[4-(3-bromophenyl)-1-piperazinyl]propyl]tetrahydro-, dihydrochloride (9CI) (CA INDEX NAME)

L12 ANSWER 1 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



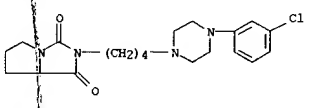
●2 HCl

RN 178482-55-8 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

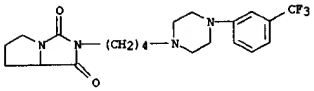
RN 178482-56-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[4-[4-(3-chlorophenyl)-1-piperazinyl]butyl]tetrahydro-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

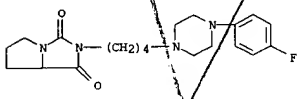
RN 178482-57-0 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]butyl]-, dihydrochloride (9CI) (CA

L12 ANSWER 1 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
INDEX NAME)



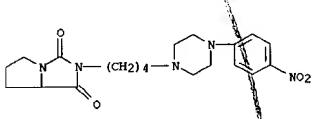
●2 HCl

RN 178482-58-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[4-[4-(4-fluorophenyl)-1-piperazinyl]butyl]tetrahydro-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

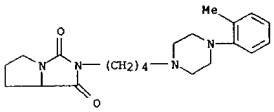
RN 178482-59-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-[4-(4-nitrophenyl)-1-piperazinyl]butyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

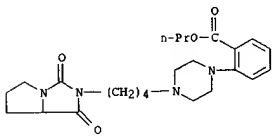
RN 178482-60-5 CAPLUS

L12 ANSWER 1 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



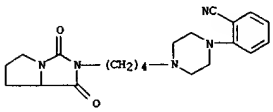
● HCl

RN 178482-63-8 CAPLUS
CN Benzoic acid, 2-[4-[4-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)butyl]-1-piperazinyl]-, propyl ester, dihydrochloride (9CI) (CA INDEX NAME)



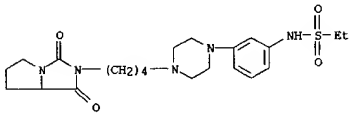
●2 HCl

L12 ANSWER 1 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
CN Benzonitrile, 2-[4-[4-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)butyl]-1-piperazinyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 178482-61-6 CAPLUS
CN Ethanesulfonamide, N-[3-[4-[4-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)butyl]-1-piperazinyl]phenyl]-, dihydrochloride (9CI)
(CA INDEX NAME)



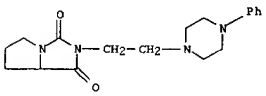
●2 HCl

RN 178482-62-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-[4-(2-methylphenyl)-1-piperazinyl]butyl]-, monohydrochloride (9CI) (CA INDEX NAME)

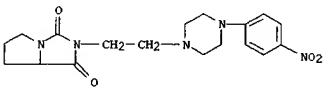
L12 ANSWER 2 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1997:309899 CAPLUS
DOCUMENT NUMBER: 126:271825
TITLE: Synthesis and Structure-Activity Relationships of a New Model of Arylpiperazines. 2. Three-Dimensional Quantitative Structure-Activity Relationships of Hydantoin-Phenylpiperazine Derivatives with Affinity for 5-HT1A and .alpha.1 Receptors. A Comparison of CoMFA Models
AUTHOR(S): Lopez-Rodriguez, Maria L.; Rosado, Ma. Luisa; Benhamu, Bellinda; Morcillo, Ma. Jose; Fernandez, Esther; Schaper, Klaus-Juergen
CORPORATE SOURCE: Departamento de Quimica Organica I Facultad de Ciencias Quimicas, Universidad Complutense, Madrid, 28040, Spain
SOURCE: J. Med. Chem. (1997), 40(11), 1648-1656
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A series of 48 bicyclohydantoin-phenylpiperazines with affinity for 5-HT1A and .alpha.1 receptors was subjected to three-dimensional quant. structure-affinity relationship anal. using comparative mol. field anal. (CoMFA), in order to get insight into the structural requirements that are responsible for 5-HT1A/.alpha.1 selectivity. Good models (high cross-validation correlations and predictive power) were obtained for 5-HT1A and .alpha.1 receptors. The resulting 3D-QSAR models rationalize steric and electrostatic factors which modulate binding to 5-HT1A and .alpha.1 receptors. A comparison of these models gives an addnl. understanding for 5-HT1A/.alpha.1 selectivity: (a) Substitution at the ortho position by a group with neg. potential is favorable to affinity for both receptors. (B) The meta position seems to be implicated in 5-HT1A/.alpha.1 selectivity. While the 5-HT1A receptor is able to accommodate bulky substituents in the region of its active site, the steric requirements of the .alpha.1 receptor are more restricted (optimum vol. of substituent 11-25 .ANG.3). (C) For both receptors the para position represents a region where the vol. accessible by the ligands is limited. (D) The hydantoin moiety and the side chain length seem to modulate not only the affinity but also 5-HT1A/.alpha.1 selectivity. The 3D-QSAR models reveal an useful predictive information for the design of new selective ligands.
IT **178482-11-6 178482-16-1 188914-65-0 188914-67-2 188914-69-4 188914-71-8**

L12 ANSWER 2 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
188914-73-0 188914-74-1 188914-83-2
188914-84-3 188914-85-4 188914-86-5
188914-94-5 188914-95-6 188914-96-7
188914-97-8 188914-98-9 188914-99-0
188915-02-8 188915-03-9 188915-04-0
188915-05-1 188915-06-2
RL: BPR (Biological process); PRP (Properties); BIOL (Biological study);
PROC (Process)
(prepn. of and affinity for 5-HT1A and .alpha.1 receptors of arylpiperazines)

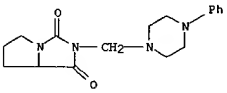
RN 178482-11-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[2-(4-phenyl-1-piperazinyl)ethyl]- (9CI) (CA INDEX NAME)



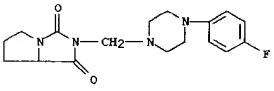
RN 178482-16-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[2-[4-(4-nitrophenyl)-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)



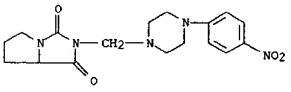
RN 188914-65-0 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[(4-phenyl-1-piperazinyl)methyl]- (9CI) (CA INDEX NAME)



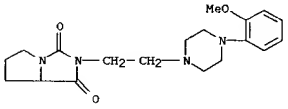
L12 ANSWER 2 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



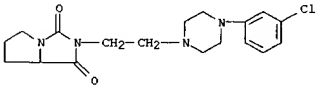
RN 188914-74-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[[4-(4-nitrophenyl)-1-piperazinyl]methyl]- (9CI) (CA INDEX NAME)



RN 188914-83-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[2-[4-(2-methoxyphenyl)-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)

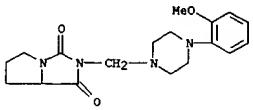


RN 188914-84-3 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[2-[4-(3-chlorophenyl)-1-piperazinyl]ethyl]tetrahydro- (9CI) (CA INDEX NAME)

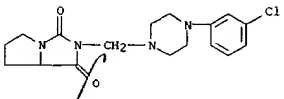


RN 188914-85-4 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[2-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)

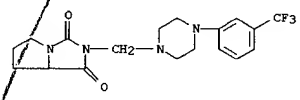
L12 ANSWER 2 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
RN 188914-67-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]- (9CI) (CA INDEX NAME)



RN 188914-69-4 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[[4-(3-chlorophenyl)-1-piperazinyl]methyl]tetrahydro- (9CI) (CA INDEX NAME)

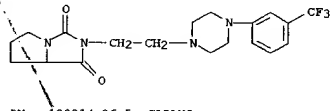


RN 188914-71-8 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]methyl]- (9CI) (CA INDEX NAME)

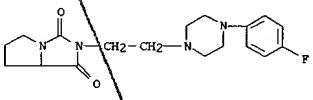


RN 188914-73-0 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[[4-(4-fluorophenyl)-1-piperazinyl]methyl]tetrahydro- (9CI) (CA INDEX NAME)

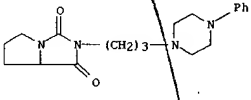
L12 ANSWER 2 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



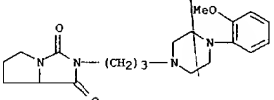
RN 188914-86-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[2-[4-(4-fluorophenyl)-1-piperazinyl]ethyl]tetrahydro- (9CI) (CA INDEX NAME)



RN 188914-94-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[3-(4-phenyl-1-piperazinyl)propyl]- (9CI) (CA INDEX NAME)

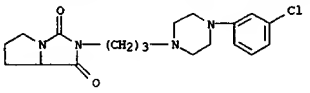


RN 188914-95-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[3-[4-(2-methoxyphenyl)-1-piperazinyl]propyl]- (9CI) (CA INDEX NAME)

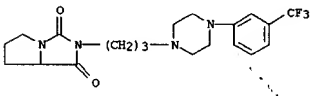


RN 188914-96-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[3-[4-(3-chlorophenyl)-1-piperazinyl]propyl]tetrahydro- (9CI) (CA INDEX NAME)

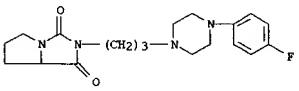
L12 ANSWER 2 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



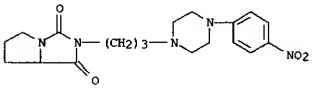
RN 188914-97-8 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[3-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]propyl]- (9CI) (CA INDEX NAME)



RN 188914-98-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[3-[4-(4-fluorophenyl)-1-piperazinyl]propyl]tetrahydro- (9CI) (CA INDEX NAME)



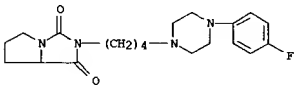
RN 188914-99-0 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[3-[4-(4-nitrophenyl)-1-piperazinyl]propyl]- (9CI) (CA INDEX NAME)



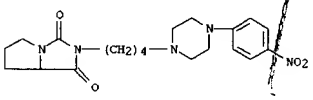
RN 188915-02-8 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-(4-phenyl-1-

L12 ANSWER 2 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

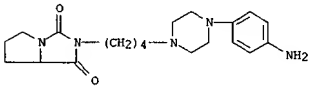
RN 188915-06-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[4-[4-(4-fluorophenyl)-1-piperazinyl]butyl]tetrahydro- (9CI) (CA INDEX NAME)



IT **188915-07-3**
RL: BPR (Biological process); PRP (Properties); RCT (Reactant); BIOL (Biological study); PROC (Process)
(prepn. of and affinity for 5-HT1A and .alpha.1 receptors of arylpiperazines)
RN 188915-07-3 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-[4-(4-nitrophenyl)-1-piperazinyl]butyl]- (9CI) (CA INDEX NAME)

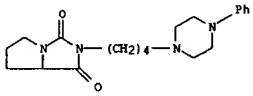


IT **188915-10-8P 188915-11-9P 188915-15-3P 188915-16-4P**
RL: BPR (Biological process); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(prepn. of and affinity for 5-HT1A and .alpha.1 receptors of arylpiperazines)
RN 188915-10-8 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[4-[4-(4-aminophenyl)-1-piperazinyl]butyl]tetrahydro- (9CI) (CA INDEX NAME)

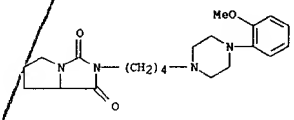


RN 188915-11-9 CAPLUS
CN Propanamide, 2-methyl-N-[3-[4-[4-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-

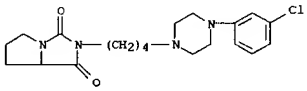
L12 ANSWER 2 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
piperazinyl)butyl]- (9CI) (CA INDEX NAME)



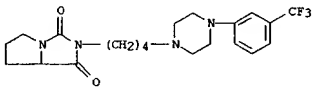
RN 188915-03-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (9CI) (CA INDEX NAME)



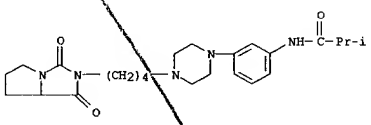
RN 188915-04-0 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[4-[4-(3-chlorophenyl)-1-piperazinyl]butyl]tetrahydro- (9CI) (CA INDEX NAME)



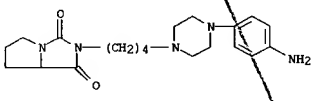
RN 188915-05-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]butyl]- (9CI) (CA INDEX NAME)



L12 ANSWER 2 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
c]imidazol-2(3H)-yl)butyl]-1-piperazinyl]phenyl]- (9CI) (CA INDEX NAME)

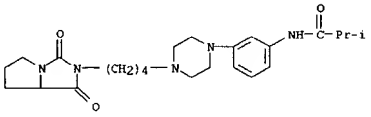


RN 188915-15-3 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[4-[4-(4-aminophenyl)-1-piperazinyl]butyl]tetrahydro-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

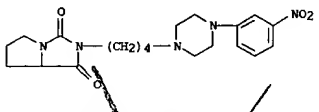
RN 188915-16-4 CAPLUS
CN Propanamide, 2-methyl-N-[3-[4-[4-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)butyl]-1-piperazinyl]phenyl]-, dihydrochloride (9CI)
(CA INDEX NAME)



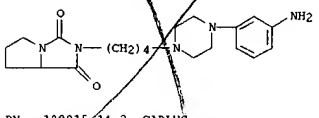
●2 HCl

IT **188915-12-0P 188915-13-1P 188915-14-2P 188916-11-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)

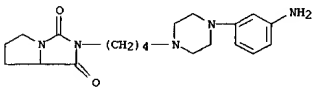
L12 ANSWER 2 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
(prepn. of and affinity for 5-HT1A and .alpha.1 receptors of arylpiperazines)
RN 188915-12-0 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-[4-(3-nitrophenyl)-1-piperazinyl]butyl]- (9CI) (CA INDEX NAME)



RN 188915-13-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[4-[4-(3-aminophenyl)-1-piperazinyl]butyl]tetrahydro- (9CI) (CA INDEX NAME)



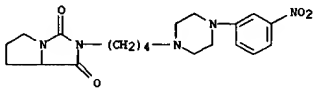
RN 188915-14-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[4-[4-(3-aminophenyl)-1-piperazinyl]butyl]tetrahydro-, trihydrochloride (9CI) (CA INDEX NAME)



●3 HCl

RN 188916-11-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-[4-(3-nitrophenyl)-1-piperazinyl]butyl]-, monohydrochloride (9CI) (CA INDEX NAME)

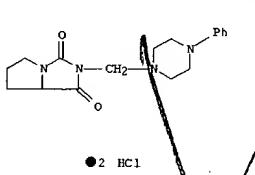
L12 ANSWER 2 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



● HCl

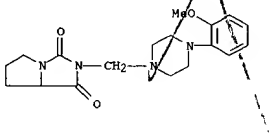
L12 ANSWER 3 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1996:601688 CAPLUS
DOCUMENT NUMBER: 125:238292
TITLE: Synthesis and Structure-Activity Relationships of a New Model of Arylpiperazines. 1. 2-[[4-(o-Methoxyphenyl)piperazin-1-yl]methyl]-1,3-dioxoperhydroimidazo[1,5-a]pyridine: A Selective 5-HT1A Receptor Agonist
AUTHOR(S): Lopez-Rodriguez, Maria L.; Rosado, M. Luisa; Benhamu, Bellinda; Morcillo, M. Jose; Sanz, Antonio M.; Orensanz, Luis; Beneitez, M. Eugenia; Fuentes, Jose A.; Manzanares, Jorge
CORPORATE SOURCE: Departamento de Quimica Organica I, Facultad de Ciencias Quimicas, Madrid, 28040, Spain
SOURCE: J. Med. Chem. (1996), 39(22), 4439-4450
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 125:238292
AB A series of new bicyclohydantoin-arylpiperazines was prepd. and evaluated for affinity at 5-HT1A, .alpha.1, and D2 receptors. Most of the compds. showed very low affinity for D2 receptors, and most of them demonstrated moderate-to-high affinity for 5-HT1A and .alpha.1 receptor binding sites. SAR observations indicated that the length of the alkyl chain between the arylpiperazine and the hydantoin moiety is of great importance for 5-HT1A/.alpha.1 affinity and selectivity, with n=1 being the optimal value. Compd. 1h, 2-[[4-(o-methoxyphenyl)piperazin-1-yl]methyl]-1,3-dioxoperhydroimidazo[1,5-a]pyridine, bound at 5-HT1A sites with nanomolar affinity (Ki = 31.7 nM) and high selectivity over .alpha.1, D2, and 5-HT2A receptors (Ki >1000, 10,000, and >1000 nM, resp.). Preliminary studies showed that this agent is probably functioning as a partial-to-full 5-HT1A agonist, and it displayed anxiolytic activity on the social interaction test in mice.
IT **178481-97-5P 178481-98-6P 178481-99-7P 178482-00-3P 178482-01-4P 178482-02-5P 178482-11-6P 178482-12-7P 178482-13-8P 178482-14-9P 178482-15-0P 178482-27-4P 178482-28-5P 178482-29-6P 178482-30-9P 178482-31-0P 178482-32-1P 178482-54-7P 178482-55-8P 178482-56-9P 178482-57-0P 178482-58-1P 178482-59-2P 181946-86-7P**
RL: BAC (Biological activity or effector, except adverse); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP

L12 ANSWER 3 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
(Preparation)
(synthesis and structure-activity relationships of new model of arylpiperazines as selective 5-HT1A receptor agonists)
RN 178481-97-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[(4-phenyl-1-piperazinyl)methyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

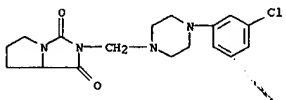
RN 178481-98-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

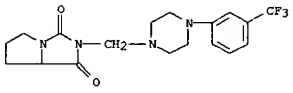
RN 178481-99-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[[4-(3-chlorophenyl)-1-piperazinyl]methyl]tetrahydro-, dihydrochloride (9CI) (CA INDEX NAME)

L12 ANSWER 3 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



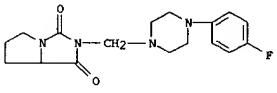
●2 HCl

RN 178482-00-3 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]methyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

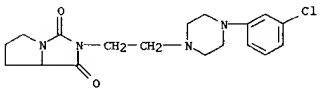
RN 178482-01-4 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[[4-(4-fluorophenyl)-1-piperazinyl]methyl]tetrahydro-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

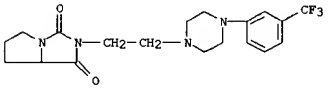
RN 178482-02-5 CAPLUS

L12 ANSWER 3 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[2-[4-(3-chlorophenyl)-1-piperazinyl]ethyl]tetrahydro-, dihydrochloride (9CI) (CA INDEX NAME)



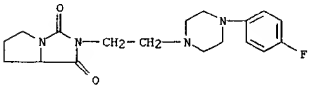
●2 HCl

RN 178482-14-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[2-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]ethyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

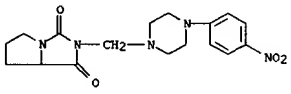
RN 178482-15-0 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[2-[4-(4-fluorophenyl)-1-piperazinyl]ethyl]tetrahydro-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

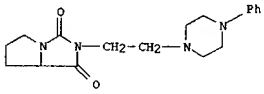
RN 178482-27-4 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[3-(4-phenyl-1-

L12 ANSWER 3 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[[4-(4-nitrophenyl)-1-piperazinyl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

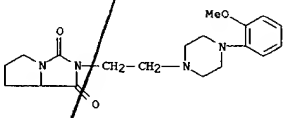


●HCl

RN 178482-11-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[2-(4-phenyl-1-piperazinyl)ethyl]- (9CI) (CA INDEX NAME)



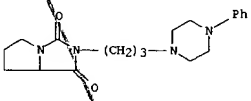
RN 178482-12-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[2-[4-(2-methoxyphenyl)-1-piperazinyl]ethyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

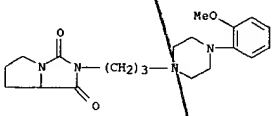
RN 178482-13-8 CAPLUS

L12 ANSWER 3 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
piperazinyl)propyl]-, dihydrochloride (9CI) (CA INDEX NAME)



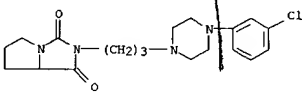
●2 HCl

RN 178482-28-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[3-[4-(2-methoxyphenyl)-1-piperazinyl]propyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

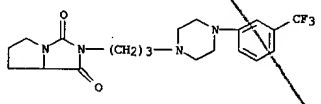
RN 178482-29-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[3-[4-(3-chlorophenyl)-1-piperazinyl]propyl]tetrahydro-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

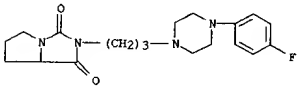
RN 178482-30-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[3-[4-[3-

L12 ANSWER 3 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
(trifluoromethyl)phenyl]-1-piperazinyl]propyl]-, dihydrochloride (9CI)
(CA INDEX NAME)



●2 HCl

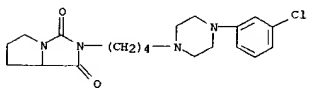
RN 178482-31-0 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[3-[4-(4-fluorophenyl)-1-piperazinyl]propyl]tetrahydro-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

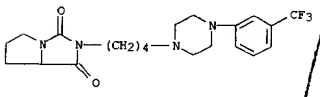
RN 178482-32-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[3-[4-(4-nitrophenyl)-1-piperazinyl]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)

L12 ANSWER 3 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[4-[4-(3-chlorophenyl)-1-piperazinyl]butyl]tetrahydro-, dihydrochloride (9CI) (CA INDEX NAME)



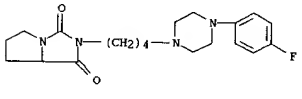
●2 HCl

RN 178482-57-0 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]butyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

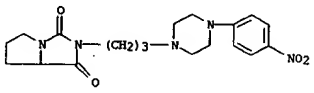
RN 178482-58-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[4-[4-(4-fluorophenyl)-1-piperazinyl]butyl]tetrahydro-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

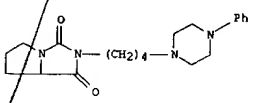
RN 178482-59-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-[4-(4-nitrophenyl)-1-piperazinyl]butyl]-, dihydrochloride (9CI) (CA INDEX NAME)

L12 ANSWER 3 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



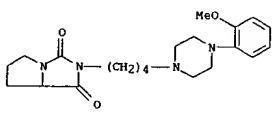
● HCl

RN 178482-54-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-(4-phenyl-1-piperazinyl)butyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

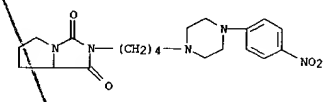
RN 178482-55-8 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

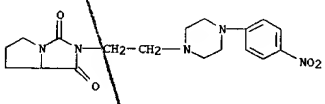
RN 178482-56-9 CAPLUS

L12 ANSWER 3 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



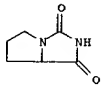
●2 HCl

RN 181948-86-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[2-[4-(4-nitrophenyl)-1-piperazinyl]ethyl]-, dihydrochloride (9CI) (CA INDEX NAME)



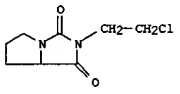
●2 HCl

IT 5768-79-6
RL: RCT (Reactant)
(synthesis and structure-activity relationships of new model of arylpiperazines as selective 5-HT1A receptor agonists)
RN 5768-79-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro- (9CI) (CA INDEX NAME)

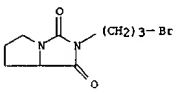


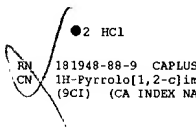
IT 178482-71-8P 181948-87-8P 181948-88-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(synthesis and structure-activity relationships of new model of arylpiperazines as selective 5-HT1A receptor agonists)
RN 178482-71-8 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(2-chloroethyl)tetrahydro-

L12 ANSWER 3 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
(9CI) (CA INDEX NAME)

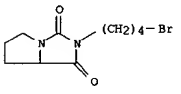


RN 181948-87-8 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione,
2-(3-bromopropyl)tetrahydro-,
dihydrochloride (9CI) (CA INDEX NAME)





RN 181948-88-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(4-bromobutyl)tetrahydro-
(9CI) (CA INDEX NAME)

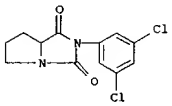


L12 ANSWER 4 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1978:22905 CAPLUS
DOCUMENT NUMBER: 88:22905
TITLE: Hydantoin and thiohydantoin derivatives
INVENTOR(S): Wakabayashi, Osamu; Matsutani, Kuni; Ota, Hiroki; Nachara, Tetsuo; Watanabe, Hisao
PATENT ASSIGNEE(S): Mitsubishi Chemical Industries Co., Ltd., Japan
SOURCE: Japan. Kokai, 12 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

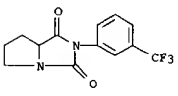
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 52083686	A2	19770712	JP 1976-224	19760101
JP 59033593	B4	19840816		

GI For diagram(s), see printed CA Issue.
AB Fifty-seven title derivs. I [Z = O, S; R = R1R2C6H3 (R1, R2 = H, alkyl, alkoxy, halo, CF3, NO2, 4-ClC6H4CH2O), .alpha.-naphthyl; n = 3, 4] were prepd. by reaction of II with RNCO or RNCS followed by dehydrative cyclization of the resulting III in the presence of acids if needed. Thus, 2.3 g 4-ClC6H4NCO in PhCl was added to an aq. mixt. of 1.94 g pipecolic acid and 0.6 g NaOH, the whole let react 4 h, washed with Et2O, acidified with HCl, and the reaction mixt. contg. a solid refluxed 1 h to give 81.1% I (Z = O, R = 4-ClC6H4, n = 4). I are useful as agricultural herbicides and fungicides; data were given against Echinochloa drug-galli, Rotana indica, Galinsoga parviflora, Digitaria adscendens, barnyard grass (millet), garden radish, Botrytis cinerea, Pellicularia sasaki, and Chochliobolus miyabeanus.
IT **60725-79-3P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and fungicidal activity of)
RN 60725-79-3 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione,
2-(3,5-dichlorophenyl)tetrahydro-
(9CI) (CA INDEX NAME)

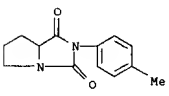
L12 ANSWER 4 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



IT **60725-54-4P 60725-55-5P 60725-56-6P**
60725-57-7P 60725-58-8P 60725-59-9P
60725-60-2P 60725-61-3P 60725-81-7P
60725-82-8P 60725-83-9P 60725-84-0P
60725-85-1P 60725-86-2P 60725-87-3P
60725-88-4P 64985-10-0P 64985-11-1P
64985-12-2P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and herbicidal activity of)
RN 60725-54-4 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

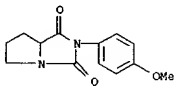


RN 60725-55-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione,
tetrahydro-2-(4-methylphenyl)-
(9CI) (CA INDEX NAME)

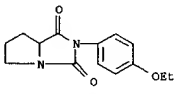


RN 60725-56-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione,
tetrahydro-2-(4-methoxyphenyl)-
(9CI) (CA INDEX NAME)

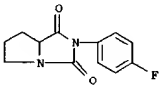
L12 ANSWER 4 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



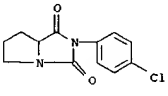
RN 60725-57-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione,
2-(4-ethoxyphenyl)tetrahydro-
(9CI) (CA INDEX NAME)



RN 60725-58-8 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione,
2-(4-fluorophenyl)tetrahydro-
(9CI) (CA INDEX NAME)

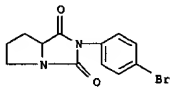


RN 60725-59-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione,
2-(4-chlorophenyl)tetrahydro-
(9CI) (CA INDEX NAME)

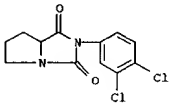


RN 60725-60-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(4-bromophenyl)tetrahydro-
(9CI) (CA INDEX NAME)

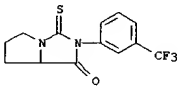
L12 ANSWER 4 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



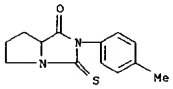
RN 60725-61-3 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(3,4-dichlorophenyl)tetrahydro- (9CI) (CA INDEX NAME)



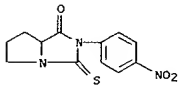
RN 60725-81-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-3-thioxo-2-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



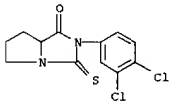
RN 60725-82-8 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-(4-methylphenyl)-3-thioxo- (9CI) (CA INDEX NAME)



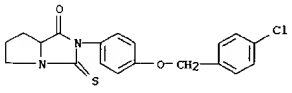
L12 ANSWER 4 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



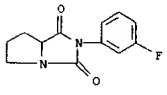
RN 60725-87-3 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(3,4-dichlorophenyl)hexahydro-3-thioxo- (9CI) (CA INDEX NAME)



RN 60725-88-4 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-[4-[(4-chlorophenyl)methoxy]phenyl]hexahydro-3-thioxo- (9CI) (CA INDEX NAME)

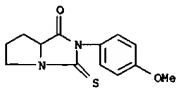


RN 64985-10-0 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(3-fluorophenyl)tetrahydro- (9CI) (CA INDEX NAME)

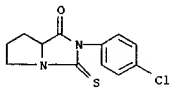


RN 64985-11-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(3-chlorophenyl)tetrahydro-

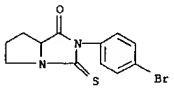
L12 ANSWER 4 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
RN 60725-83-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-(4-methoxyphenyl)-3-thioxo- (9CI) (CA INDEX NAME)



RN 60725-84-0 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(4-chlorophenyl)hexahydro-3-thioxo- (9CI) (CA INDEX NAME)

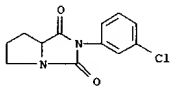


RN 60725-85-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(4-bromophenyl)hexahydro-3-thioxo- (9CI) (CA INDEX NAME)

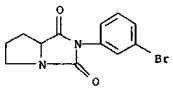


RN 60725-86-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-(4-nitrophenyl)-3-thioxo- (9CI) (CA INDEX NAME)

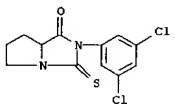
L12 ANSWER 4 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
(9CI) (CA INDEX NAME)



RN 64985-12-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(3-bromophenyl)tetrahydro- (9CI) (CA INDEX NAME)



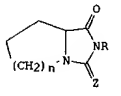
IT **60726-07-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and herbicidal and fungicidal activities of)
RN 60726-07-0 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(3,5-dichlorophenyl)hexahydro-3-thioxo- (9CI) (CA INDEX NAME)



L12 ANSWER 5 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1980:446672 CAPLUS
DOCUMENT NUMBER: 93:46672
TITLE: 1,5-Alkylene-3-arylhydantoin derivatives
PATENT ASSIGNEE(S): Mitsubishi Chemical Industries Co., Ltd., Japan
SOURCE: Brit. Amended B, 30 pp.
CODEN: BSXXBI
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

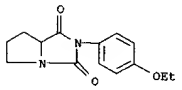
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1503244	A	19780308	GB 1976-5128	19760210
JP 51095134	A2	19760820	JP 1975-16211	19750210
JP 52042877	A2	19770404	JP 1975-118035	19750930
JP 52042893	A2	19770404	JP 1975-118036	19750930
CA 1076114	A1	19800422	CA 1976-245153	19760205
NL 7601296	A	19760812	NL 1976-1296	19760209
FR 2300083	A1	19760903	FR 1976-3459	19760209
FR 2300083	B1	19790504		
CH 624272	A	19810731	CH 1976-1532	19760209
PRIORITY APPLN. INFO.:			JP 1975-16211	19750210
			JP 1975-118035	19750930
			JP 1975-118036	19750930

GI

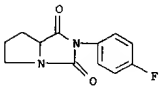


AB Fifty-seven title compds. I (n = 1, 2; Z = O, S; R = Ph substituted by
.gtoreq.1 halo, alkyl, alkoxy, NO2, haloalkyl, halobenzyloxy, naphthyl),
useful as fungicides and herbicides, were prepd. from substituted imino
acids or their esters by cyclization or reaction with aryl isocyanates or
isothiocyanates. Thus, I (n = 1, Z = O, R = 3-CF3C6H4) was prepd. (92.2%)
from N-[N'-(m-trifluoromethylphenyl)carbamoyl]proline by heating with 2N
HCl and dioxane at reflux for 2 h. The herbicidal and fungicidal activities of I were assessed. Compns. contg. I are described.

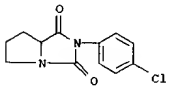
L12 ANSWER 5 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
(9CI) (CA INDEX NAME)



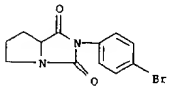
RN 60725-58-8 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(4-fluorophenyl)tetrahydro-
(9CI) (CA INDEX NAME)



RN 60725-59-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(4-chlorophenyl)tetrahydro-
(9CI) (CA INDEX NAME)

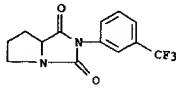


RN 60725-60-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(4-bromophenyl)tetrahydro-
(9CI) (CA INDEX NAME)

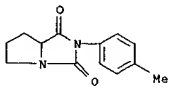


RN 60725-61-3 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(3,4-dichlorophenyl)tetrahydro-

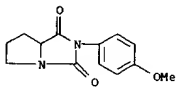
L12 ANSWER 5 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
IT 60725-54-4P 60725-55-5P 60725-56-6P
60725-57-7P 60725-58-8P 60725-59-9P
60725-60-2P 60725-61-3P 60725-79-3P
60725-82-8P 60725-83-9P 60725-84-0P
60725-85-1P 60725-86-2P 60725-87-3P
60725-88-4P 60726-07-0P 74142-17-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as fungicide and herbicide)
RN 60725-54-4 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 60725-55-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-(4-methylphenyl)-
(9CI) (CA INDEX NAME)

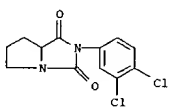


RN 60725-56-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-(4-methoxyphenyl)-
(9CI) (CA INDEX NAME)

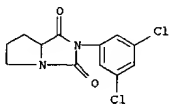


RN 60725-57-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(4-ethoxyphenyl)tetrahydro-

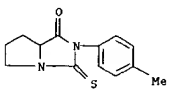
L12 ANSWER 5 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
(9CI) (CA INDEX NAME)



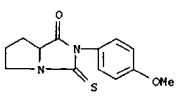
RN 60725-79-3 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(3,5-dichlorophenyl)tetrahydro-
(9CI) (CA INDEX NAME)



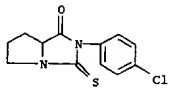
RN 60725-82-8 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-(4-methylphenyl)-3-thioxo-
(9CI) (CA INDEX NAME)



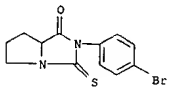
RN 60725-83-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-(4-methoxyphenyl)-3-thioxo-
(9CI) (CA INDEX NAME)



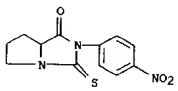
L12 ANSWER 5 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
RN 60725-84-0 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(4-chlorophenyl)hexahydro-3-thioxo- (9CI) (CA INDEX NAME)



RN 60725-85-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(4-bromophenyl)hexahydro-3-thioxo- (9CI) (CA INDEX NAME)

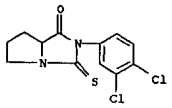


RN 60725-86-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-(4-nitrophenyl)-3-thioxo- (9CI) (CA INDEX NAME)

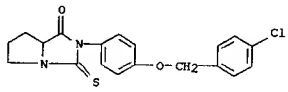


RN 60725-87-3 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(3,4-dichlorophenyl)hexahydro-3-thioxo- (9CI) (CA INDEX NAME)

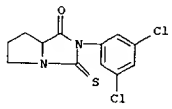
L12 ANSWER 5 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



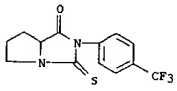
RN 60725-88-4 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-[4-[(4-chlorophenyl)methoxy]phenyl]hexahydro-3-thioxo- (9CI) (CA INDEX NAME)



RN 60726-07-0 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(3,5-dichlorophenyl)hexahydro-3-thioxo- (9CI) (CA INDEX NAME)



RN 74142-17-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-3-thioxo-2-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



L12 ANSWER 5 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

L12 ANSWER 6 OF 208 CAPLUS COPYRIGHT 2001 ACS

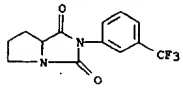
ACCESSION NUMBER: 1976:560100 CAPLUS
DOCUMENT NUMBER: 85:160100
TITLE: Herbicidal and fungicidal 1,5-alkylen-3-aryl hydantoin derivatives
INVENTOR(S): Wakabayashi, Osamu; Matsuya, Kuni; Ohta, Hiroki; Jikihara, Tetsuo; Watanabe, Hisao
PATENT ASSIGNEE(S): Mitsubishi Chemical Industries Co., Ltd., Japan
SOURCE: Ger. Offen., 49 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2604989	A1	19760819	DE 1976-2604989	19760209
JP 51095134	A2	19760820	JP 1975-16211	19750210
JP 52042877	A2	19770404	JP 1975-118035	19750930
JP 52042893	A2	19770404	JP 1975-118036	19750930
CA 1076114	A1	19800422	CA 1976-245153	19760205
NL 7601296	A	19760812	NL 1976-1296	19760209
FR 2300083	A1	19760903	FR 1976-3459	19760209
FR 2300083	B1	19790504		
CH 624272	A	19810731	CH 1976-1532	19760209

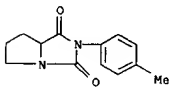
PRIORITY APPLN. INFO.: JP 1975-16211 19750210
JP 1975-118035 19750930
JP 1975-118036 19750930

GI For diagram(s), see printed CA Issue.
AB Hydantoin derivs. [I; Rn = e.g., 4-Br, 4-Cl, 4-F, 4-Me, 4-MeO, 3-F3C, 3,5-Cl2, 4,3-ClMe; Q = (CH2)3, (CH2)4; X = O, S], with fungicidal and herbicidal activity, are prepd. by cyclization of N-(phenylcarbamoyl) derivs. of 2-piperidine- and 2-pyrrolidinecarboxylic acid. The carbamoyl derivs. are obtained by reaction of the appropriately substituted Ph isocyanate or isothiocyanate with the acids or their Me or Et esters. Thus, cyclization of 1-[3-(trifluoromethyl)phenyl]-2-pyrrolidinecarboxylic acid, prepd. from proline and m-(F3C)C6H4NCO, for 2 hr in refluxing dioxane in presence of HCl gives 92.2% I [Rn = 3-F3C, Q = (CH2)3, X = O].
IT **60725-54-4P 60725-55-5P 60725-56-6P**
60725-57-7P 60725-58-8P 60725-59-9P
60725-60-2P 60725-61-3P 60725-79-3P
60725-81-7P 60725-82-8P 60725-83-9P
60725-84-0P 60725-85-1P 60725-86-2P
60725-87-3P 60725-88-4P 60726-07-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and fungicidal and herbicidal activity of)
RN 60725-54-4 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

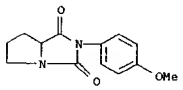
L12 ANSWER 6 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



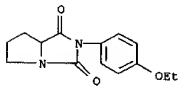
RN 60725-55-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-(4-methylphenyl)- (9CI) (CA INDEX NAME)



RN 60725-56-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

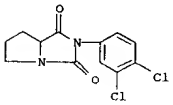


RN 60725-57-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(4-ethoxyphenyl)tetrahydro- (9CI) (CA INDEX NAME)

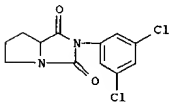


RN 60725-58-8 CAPLUS

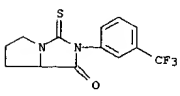
L12 ANSWER 6 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



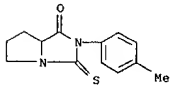
RN 60725-79-3 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(3,5-dichlorophenyl)tetrahydro- (9CI) (CA INDEX NAME)



RN 60725-81-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-3-thioxo-2-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

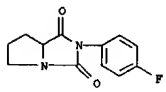


RN 60725-82-8 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-(4-methylphenyl)-3-thioxo- (9CI) (CA INDEX NAME)

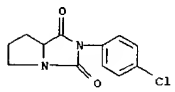


RN 60725-83-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-(4-methoxyphenyl)-3-thioxo-

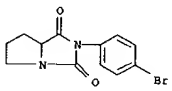
L12 ANSWER 6 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(4-fluorophenyl)tetrahydro- (9CI) (CA INDEX NAME)



RN 60725-59-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(4-chlorophenyl)tetrahydro- (9CI) (CA INDEX NAME)

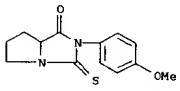


RN 60725-60-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(4-bromophenyl)tetrahydro- (9CI) (CA INDEX NAME)

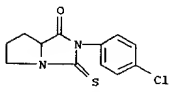


RN 60725-61-3 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(3,4-dichlorophenyl)tetrahydro- (9CI) (CA INDEX NAME)

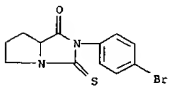
L12 ANSWER 6 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
(9CI) (CA INDEX NAME)



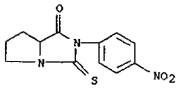
RN 60725-84-0 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(4-chlorophenyl)hexahydro-3-thioxo- (9CI) (CA INDEX NAME)



RN 60725-85-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(4-bromophenyl)hexahydro-3-thioxo- (9CI) (CA INDEX NAME)

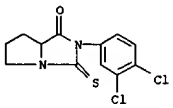


RN 60725-86-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-(4-nitrophenyl)-3-thioxo- (9CI) (CA INDEX NAME)

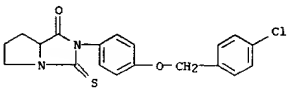


RN 60725-87-3 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(3,4-dichlorophenyl)hexahydro-3-thioxo- (9CI) (CA INDEX NAME)

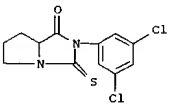
L12 ANSWER 6 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



RN 60725-88-4 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-[4-[(4-chlorophenyl)methoxy]phenyl]hexahydro-3-thioxo- (9CI) (CA INDEX NAME)

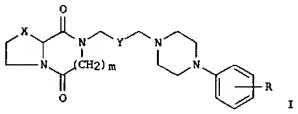


RN 60726-07-0 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(3,5-dichlorophenyl)hexahydro-3-thioxo- (9CI) (CA INDEX NAME)



L12 ANSWER 7 OF 208 CAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 2000:892727 CAPLUS
DOCUMENT NUMBER: 134:207793
TITLE: Synthesis and Structure-Activity Relationships of a New Model of Arylpiperazines. 5.Study of the Physicochemical Influence of the Pharmacophore on 5-HT1A/.alpha.1-Adrenergic Receptor Affinity: Synthesis of a New Derivative with Mixed 5-HT1A/D2 Antagonist Properties
AUTHOR(S): Lopez-Rodriguez, Maria L.; Morcillo, M. Jose; Fernandez, Esther; Porras, Esther; Orensanz, Luis; Beneytez, M. Eugenia; Manzanares, Jorge; Fuentes, Jose Angel
CORPORATE SOURCE: Departamento de Quimica Organica I Facultad de Ciencias Quimicas and Departamento de Farmacologia Facultad de Farmacia, Universidad Complutense, Madrid, 28040, Spain
SOURCE: J. Med. Chem. (2001), 44(2), 186-197
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

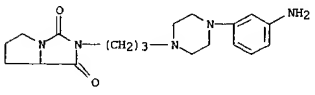
AB A test series of 32 amide arylpiperazines I (m = 0, 1; X, Y = CH2, CH2CH2; R = 2-Me, 2-MeO, 2-CN, 3-CF3, 3-NH2, 3-Br, etc.) has been prepd. in order to gain insight into the physicochem. influence of the pharmacophores of 5-HT1A and .alpha.1-adrenergic receptors. The training set was designed applying a fractional factorial design using six physicochem. descriptors. The amide moiety is a bicyclohydantoin or a diketopiperazine, the spacer length is 3 or 4 methylene units, which are the optimum values for both

L12 ANSWER 7 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

receptors, and the arom. substituent R occupies the ortho- or meta-position and has been selected from a database of 387 substituents using the EDISFAR program. The 5-HT1A and .alpha.1-adrenergic receptor binding affinities of synthesized compds. have been detd. This data set has been used to derive classical quant. structure-activity relationships (QSAR) and neural networks models for both receptors. A comparison of these models gives information for the design of the new ligand EF-7412 I (m = 0; X = CH2; Y = CH2CH2; R = 3-EtSO2NH) (II) (5-HT1A: Ki = 27 nM; .alpha.1: Ki > 1000 nM). II displays affinity for the dopamine D2 receptor (Ki = 22 nM) and is selective vs. all other receptors examd. (5-HT2A, 5-HT3, 5-HT4 and Bz; Ki > 1000 nM). II acts as an antagonist in vivo in pre- and postsynaptic 5-HT1A receptor sites and as an antagonist in the dopamine D2 receptor. Thus, II is a deriv. with mixed 5-HT1A/D2 antagonist properties and this deriv. could be useful as a pharmacol. tool.

IT **178482-35-4P**
RL: BAC (Biological activity or effector, except adverse); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and structure-activity relationships of arylpiperazines as antagonists of adrenergic and dopamine receptors)

RN 178482-35-4 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[3-[4-(3-aminophenyl)-1-piperazinyl]propyl]tetrahydro-, dihydrochloride (9CI) (CA INDEX NAME)

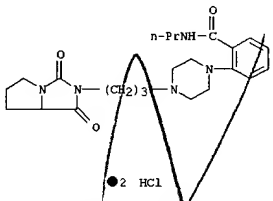


●2 HCl

IT **178482-33-2P 178482-34-3P 178482-36-5P**
178482-60-5P 178482-61-6P 178482-62-7P
188915-16-4P 328410-12-4P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

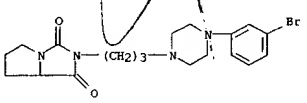
L12 ANSWER 7 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
(prepn. and structure-activity relationships of arylpiperazines as antagonists of adrenergic and dopamine receptors)

RN 178482-33-2 CAPLUS
CN Benzamide, N-propyl-2-[4-[3-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)propyl]-1-piperazinyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

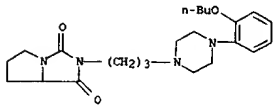
RN 178482-34-3 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[3-[4-(3-bromophenyl)-1-piperazinyl]propyl]tetrahydro-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

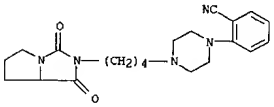
RN 178482-36-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[3-[4-(2-butoxyphenyl)-1-piperazinyl]propyl]tetrahydro-, dihydrochloride (9CI) (CA INDEX NAME)

L12 ANSWER 7 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



●2 HCl

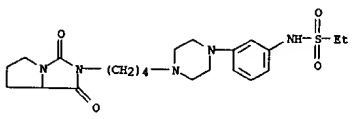
RN 178482-60-5 CAPLUS
CN Benzonitrile, 2-[4-[4-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)butyl]-1-piperazinyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

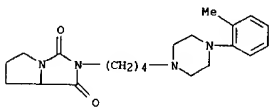
RN 178482-61-6 CAPLUS
CN Ethanesulfonamide, N-[3-[4-[4-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)butyl]-1-piperazinyl]phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)

L12 ANSWER 7 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



●2 HCl

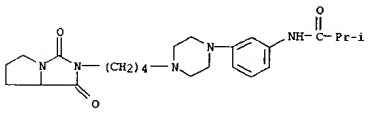
RN 178482-62-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-[4-(2-methylphenyl)-1-piperazinyl]butyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

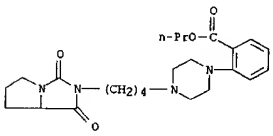
RN 188915-16-4 CAPLUS
CN Propanamide, 2-methyl-N-[3-[4-[4-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)butyl]-1-piperazinyl]phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)

L12 ANSWER 7 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



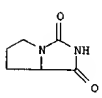
●2 HCl

RN 328410-12-4 CAPLUS
CN Benzoic acid, 2-[4-[4-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)butyl]-1-piperazinyl]-, propyl ester, monohydrochloride (9CI) (CA INDEX NAME)



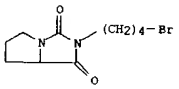
● HCl

IT **5768-79-6 181948-88-9**
RL: RCT (Reactant)
(prepn. and structure-activity relationships of arylpiperazines as antagonists of adrenergic and dopamine receptors)
RN 5768-79-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro- (9CI) (CA INDEX NAME)

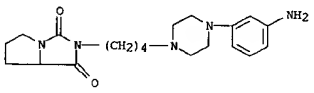


L12 ANSWER 7 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

RN 181948-88-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(4-bromobutyl)tetrahydro- (9CI) (CA INDEX NAME)

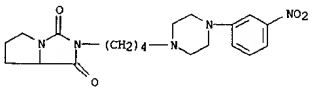


IT **188915-14-2P 188916-11-2P 328410-06-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and structure-activity relationships of arylpiperazines as antagonists of adrenergic and dopamine receptors)
RN 188915-14-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[4-[4-(3-aminophenyl)-1-piperazinyl]butyl]tetrahydro-, trihydrochloride (9CI) (CA INDEX NAME)



●3 HCl

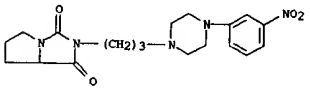
RN 188916-11-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-[4-(3-nitrophenyl)-1-piperazinyl]butyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 328410-06-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[3-[4-(3-

L12 ANSWER 7 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
nitrophenyl)-1-piperazinyl]propyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 41
REFERENCE(S):
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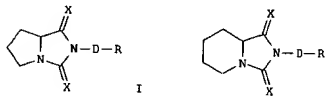
(2) Ahlenius, S; Eur Neuropsychopharmacol 1999, V9, P15 CAPLUS
(3) Ambrosio, E; Neurosci Lett 1984, V49, P193 CAPLUS
(5) Armario, A; Rev Esp Fisiol 1984, V40, P437 CAPLUS
(9) Cheng, Y; Biochem Pharmacol 1973, V22, P3099 CAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 8 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 2001:472720 CAPLUS
DOCUMENT NUMBER: 135:76872
TITLE: Preparation of hydantoin derivatives for preventing and/or treating neurological disorders
PATENT ASSIGNEE(S): GPI NIL Holdings, Inc., USA
SOURCE: PCT Int. Appl., 99 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001046195	A1	20010628	WO 2000-US30436	20001106

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

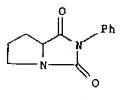
PRIORITY APPLN. INFO.: US 1999-171391 P 19991221
OTHER SOURCE(S): MARPAT 135:76872
GI



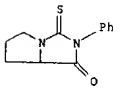
I II

AB The title compds. [I or II; X = O, S, NR2; R2 = CN, NO2, H, etc.; D = a

L12 ANSWER 8 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
direct bond, alkyl, alkenyl; R = H, Ph, biphenyl, etc.], useful in preventing and/or treating neurol. disorders, including phys. damaged nerves and neurodegenerative diseases, for treating alopecia and promoting hair growth, for treating vision disorders and/or improving vision, for treating memory impairment and/or enhancing memory performance, and for treating sensorineural hearing loss, were prepd. and formulated. Thus, reacting L-proline Me ester with phenylethyl isothiocyanate in the presence of Et3N in CH2Cl2 afforded I [X1 = S; X2 = O; D = (CH2)2; R = Ph] which showed 42.50% recovery of dopaminergic neurons in MPTP model of Parkinson's disease in mice. Biol. data show remarkable neuroregenerative effects of compds. I illustrating their neurotrophic capability.
IT **2221-09-2P 4333-21-5P 346688-05-9P 346688-08-2P 346688-09-3P 346688-11-7P 346688-13-9P 346688-15-1P 346688-17-3P 346688-19-5P 346688-26-4P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of hydantoin derivs. for preventing and/or treating neurol. disorders)
RN 2221-09-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-phenyl- (9CI) (CA INDEX NAME)

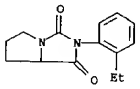


RN 4333-21-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo- (9CI) (CA INDEX NAME)



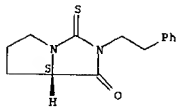
L12 ANSWER 8 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

RN 346688-05-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(2-ethylphenyl)tetrahydro- (9CI) (CA INDEX NAME)

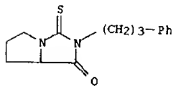


RN 346688-08-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-(2-phenylethyl)-3-thioxo-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



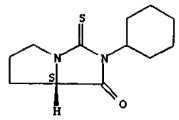
RN 346688-09-3 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-(3-phenylpropyl)-3-thioxo- (9CI) (CA INDEX NAME)



RN 346688-11-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-cyclohexylhexahydro-3-thioxo-, (7aS)- (9CI) (CA INDEX NAME)

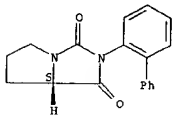
Absolute stereochemistry.

L12 ANSWER 8 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



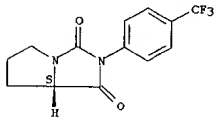
RN 346688-13-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[1,1'-biphenyl]-2-yltetrahydro-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 346688-15-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-(trifluoromethyl)phenyl]-, (7aS)- (9CI) (CA INDEX NAME)

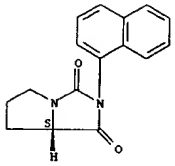
Absolute stereochemistry.



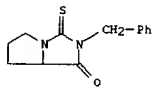
RN 346688-17-3 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-(1-naphthalenyl)-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

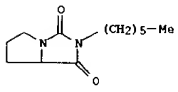
L12 ANSWER 8 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



RN 346688-19-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-(phenylmethyl)-3-thioxo- (9CI) (CA INDEX NAME)



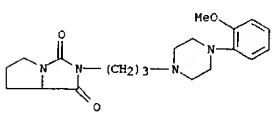
RN 346688-26-4 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-hexyltetrahydro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 9
REFERENCE(S):
(1) Aizenman; US 5145862 A 1992 CAPLUS
(3) Jamieson; US 4230709 A 1980 CAPLUS
(4) Liao, Z; JOURNAL OF ORGANIC CHEMISTRY 1984, V49(25), P4745 CAPLUS
(6) Mochida; US 5232936 A 1993 CAPLUS
(7) Proctor; WO 8805653 A 1988 CAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

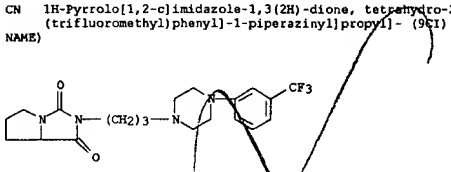
L12 ANSWER 8 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

L12 ANSWER 9 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1997:528590 CAPLUS
DOCUMENT NUMBER: 127:130461
TITLE: Synthesis and Structure-Activity Relationships of a New Model of Arylpiperazines. 3. 2-[.omega.-(4-Arylpiperazin-1-yl)alkyl]perhydropyrrolo[1,2-c]imidazol s and -pechydroimidazo[1,5-a]pyridines: Study of the Influence of the Terminal Amide Fragment on 5-HT1A Affinity/Selectivity
AUTHOR(S): Lopez-Rodriguez, Maria L.; Morcillo, M. Jose; Fernandez, Esther; Porras, Esther; Murcia, Marta; Sanz, Antonio M.; Orensanz, Luis
CORPORATE SOURCE: Departamento de Quimica Organica I Facultad de Ciencias Quimicas, Universidad Complutense, Madrid, 28040, Spain
SOURCE: J. Med. Chem. (1997), 40(16), 2653-2656
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A series of new arylpiperazine derivs., which are devoid of the terminal amide fragment present in related 5-HT1A ligands, was prepd. and evaluated for affinity at 5-HT1A and .alpha.1 receptors. All the compds. demonstrated high affinity for the 5-HT1A receptor and moderate affinity for .alpha.1 receptor binding sites. Structure-activity relationship (SAR) studies suggest that there is influence of electronic factors on the no-pharmacophoric part of the .alpha.1 receptor site. However there is no influence of electronic interactions on the stabilization of the 5-HT1A receptor-ligand complex.
IT **188914-95-6 188914-97-8 188915-03-9 188915-04-0 188915-05-1**
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(affinity at .alpha.1- and 5-HT1A-receptors of arylpiperazines)
RN 188914-95-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[3-[4-(2-methoxyphenyl)-1-piperazinyl]propyl]- (9CI) (CA INDEX NAME)

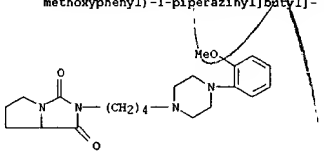


L12 ANSWER 9 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

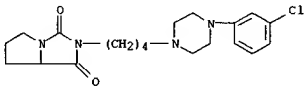
RN 188914-97-8 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[3-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]propyl]- (9CI) (CA INDEX NAME)



RN 188915-03-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-[4-(2-methoxyphenyl)-1-piperazinyl]butyl]- (9CI) (CA INDEX NAME)

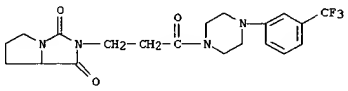


RN 188915-04-0 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[4-[4-(3-chlorophenyl)-1-piperazinyl]butyl]tetrahydro- (9CI) (CA INDEX NAME)

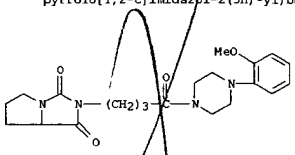


RN 188915-05-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]butyl]- (9CI) (CA INDEX NAME)

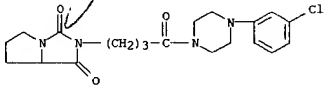
L12 ANSWER 9 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



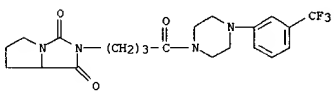
RN 192993-02-5 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[1-oxo-4-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)butyl]- (9CI) (CA INDEX NAME)



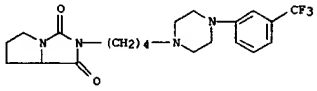
RN 192993-03-6 CAPLUS
CN Piperazine, 1-(3-chlorophenyl)-4-[1-oxo-4-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)butyl]- (9CI) (CA INDEX NAME)



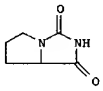
RN 192993-04-7 CAPLUS
CN Piperazine, 1-[1-oxo-4-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)butyl]-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



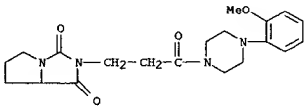
L12 ANSWER 9 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



IT **5768-79-6**
RL: RCT (Reactant)
(prepn. and affinity at .alpha.1- and 5-HT1A-receptors of arylpiperazines)
RN 5768-79-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro- (9CI) (CA INDEX NAME)



IT **192992-97-5P 192992-98-6P 192993-02-5P 192993-03-6P 192993-04-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and affinity at .alpha.1- and 5-HT1A-receptors of arylpiperazines)
RN 192992-97-5 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[1-oxo-3-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)propyl]- (9CI) (CA INDEX NAME)



RN 192992-98-6 CAPLUS
CN Piperazine, 1-[1-oxo-3-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)propyl]-4-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

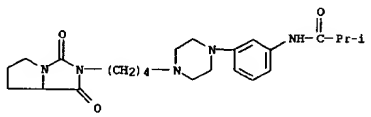
L12 ANSWER 10 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 2000:897084 CAPLUS
DOCUMENT NUMBER: 134:172689
TITLE: Synthesis and Structure-Activity Relationships of a New Model of Arylpiperazines. 6. Study of the 5-HT1A/.alpha.1-Adrenergic Receptor Affinity by Classical Hansch Analysis, Artificial Neural Networks, and Computational Simulation of Ligand Recognition
AUTHOR(S): Lopez-Rodriguez, Maria L.; Morcillo, M. Jose; Fernandez, Esther; Rosado, M. Luisa; Pardo, Leonardo; Schaper, Klaus-Juergen
CORPORATE SOURCE: Departamento de Quimica Organica I Facultad de Ciencias Quimicas, Universidad Complutense, Madrid, 28040, Spain
SOURCE: J. Med. Chem. (2001), 44(2), 198-207
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A classical quant. structure-activity relationship (Hansch) study and artificial neural networks (ANNs) have been applied to a training set of 32 substituted phenylpiperazines with affinity for 5-HT1A and .alpha.1-adrenergic receptors, to evaluate the structural requirements that are responsible for 5-HT1A/.alpha.1 selectivity. The resulting models provide a significant correlation of electronic, steric, and hydrophobic parameters with the biol. affinities. Although the derived linear Hansch correlations give good statistics and acceptable predictions, the introduction of nonlinear relationships in the anal. gives more solid models and more accurate predictions. In the ANN models on the basis of the obtained 3D plots, the 5-HT1A affinity has a nonlinear dependence on F, Vo, Vm, and .pi.o, although the nonlinear relationship is not far from a planar one. The .alpha.1-adrenergic receptor affinity has a clear nonlinear dependence on F, Vo, Vm, .pi.o, and .pi.m. A comparison of both analyses gives an addnl. understanding for 5-HT1A/.alpha.1 selectivity: (a) high F values increase the binding affinity for 5-HT1A receptors and decrease the affinity for .alpha.1 sites; (b) the hydrophobicity at the meta-position has only influence for the .alpha.1-adrenergic receptor; (c) the meta-position seems to be implicated in the 5-HT1A/.alpha.1 selectivity. While the 5-HT1A receptor is able to accommodate bulky substituents in the region of its active site, the steric requirements of the .alpha.1-adrenergic receptor at this position

L12 ANSWER 10 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
are more restricted. This information was used for the design of the new
ligand EF-7412 (33) (5-HT1A: Ki exptl = 27 nM, .alpha.1: Ki exptl > 1000
nM; 5-HT1A:Ki pred ANN = 36 nM, .alpha.1: Ki pred ANN = 2745 nM) which was
characterized as an antagonist in vivo in pre- and postsynaptic 5-HT1AR
sites. Computational simulations of the complex between EF-7412 (33) and
a 3D model of the transmembrane domain of the 5-HT1A receptor allowed us
to define the mol. details of the ligand-receptor interaction that
includes: (i) the ionic interaction between the protonated amine of the
ligand and Asp 3.32; (ii) the hydrogen bonds between the m-NHSO2Et group
of the ligand and Asn 7.39; and the hydrogen bonds between the hydantoin
moiety of the ligand and (iii) Thr 3.37, (iv) Ser 5.42, and (v) Thr 5.43.
These QSAR and ANN results in combination with computational simulations
of ligand recognition will be useful for the design of potent selective
5-HT1A ligands.

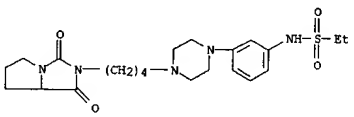
IT **188915-11-9 221452-76-2**, EF-7412 **326497-29-4**
326497-30-7 326497-31-8 326497-33-0
326497-46-5 326497-47-6 326497-48-7
RL: BAC (Biological activity or effector, except adverse); PRP (Properties); BIOL (Biological study)
(synthesis and structure-activity relationships of arylpiperazines with
affinity for 5-HT1A and .alpha.1-adrenergic receptors, classical hansch
anal., artificial neural networks, and computational simulation of ligand recognition)

RN 188915-11-9 CAPLUS
CN Propanamide, 2-methyl-N-[3-[4-[4-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)butyl]-1-piperazinyl]phenyl]- (9CI) (CA INDEX NAME)

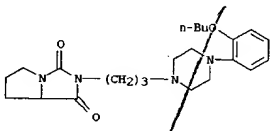
L12 ANSWER 10 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



RN 221452-76-2 CAPLUS
CN Ethanesulfonamide, N-[3-[4-[4-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)butyl]-1-piperazinyl]phenyl]- (9CI) (CA INDEX NAME)

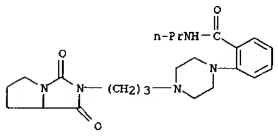


RN 326497-29-4 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[3-[4-(2-butoxyphenyl)-1-piperazinyl]propyl]tetrahydro- (9CI) (CA INDEX NAME)

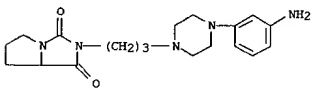


RN 326497-30-7 CAPLUS
CN Benzamide, N-propyl-2-[4-[3-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)propyl]-1-piperazinyl]- (9CI) (CA INDEX NAME)

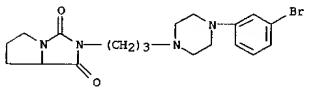
L12 ANSWER 10 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



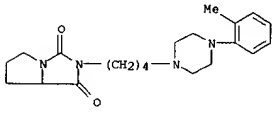
RN 326497-31-8 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[3-[4-(3-aminophenyl)-1-piperazinyl]propyl]tetrahydro- (9CI) (CA INDEX NAME)



RN 326497-33-0 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[3-[4-(3-bromophenyl)-1-piperazinyl]propyl]tetrahydro- (9CI) (CA INDEX NAME)



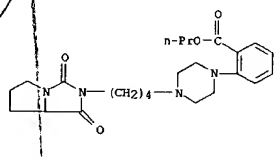
RN 326497-46-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-[4-(2-methylphenyl)-1-piperazinyl]butyl]- (9CI) (CA INDEX NAME)



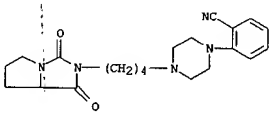
RN 326497-47-6 CAPLUS

L12 ANSWER 10 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

CN Benzoic acid, 2-[4-[4-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)butyl]-1-piperazinyl]-, propyl ester (9CI) (CA INDEX NAME)



RN 326497-48-7 CAPLUS
CN Benzonitrile, 2-[4-[4-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)butyl]-1-piperazinyl]- (9CI) (CA INDEX NAME)

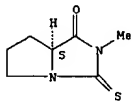


REFERENCE COUNT: 39
REFERENCE(S): (1) Ambrosio, E; Neurosci Lett 1984, V49, P193 CAPLUS
(2) Andrea, T; J Med Chem 1991, V34, P2824 CAPLUS
(3) Aoyama, T; Chem Pharm Bull 1991, V39, P1222 CAPLUS
(4) Ballesteros, J; Methods Neurosci 1995, V25, P366
CAPLUS
(6) Bourne, H; Science 2000, V289, P733 CAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 11 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1996:110170 CAPLUS
DOCUMENT NUMBER: 124:277362
TITLE: Reversed phase planar chromatography of enantiomeric compounds on microcrystalline triacetyl cellulose
AUTHOR(S): Lepri, Luciano
CORPORATE SOURCE: Dep. of Public Health, Epidemiology, and Environ. Analytical Chemistry, Univ. of Florence, Florence, 50121, Italy
SOURCE: J. Planar Chromatogr.--Mod. TLC (1995), 8(6), 467-9
CODEN: JPCTE5; ISSN: 0933-4173
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The aim of this work was to verify the resolving ability of microcryst. cellulose triacetate (MCTA) towards new structurally related racemates and to achieve further information about the contribution of the shape of the mol. and the polarity and the steric effects of the groups close to the asym. C, to chiral recognition. Retention and resoln. data for enantiomeric compds. on MCTA plates with silica gel 60 GF254 as binder are given. A TLC of several racemates, pure optical isomers, and their mixts. on MCTA eluted with iso-PrOH-H2O, 60:40 (vol./vol.) at 25.degree. is presented: (.+-.)-2-phenylbutyrophenone (a); R-(+)-1,1,2-triphenyl-1,2-ethanediol (b); S-(-)-1,1,2-triphenyl-1,2-ethanediol (c); mixt. of (b) and (c); (2S)-(-)-3,3-dimethylglycidyl-4-nitrobenzoate (d); (2R)-(+)-3,3-dimethylglycidyl-4-nitrobenzoate (e); mixt. of (d) and (e); (.+-.)-carprofen; (S)-(-)-4-benzyl-2-oxazolidinone; (R)-(7)-4-benzyl-2-oxazolidinone; MTH-DL-Phe, MTH-DL-Tyr; MTH-DL-Pro; MTH-DL-Trp; MTH-DL-Leu; and PTH-DL-Trp. The role of the chem. characteristics of the solutes in chiral recognition was also addressed.
IT **1968-34-9 28868-23-7 29635-99-2 31364-82-6 145552-40-5 175274-20-1**
RL: ANT (Analyte); PEP (Physical, engineering or chemical process); ANST (Analytical study); PROC (Process)
(reversed phase planar chromatog. of enantiomeric compds. on microcryst. triacetyl cellulose)
RN 1968-34-9 CAPLUS

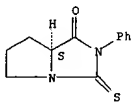
L12 ANSWER 11 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
RN 28868-23-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



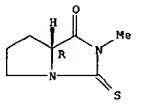
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 31364-82-6 CAPLUS
RN 145552-40-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo-, (7aR)-(9CI) (CA INDEX NAME)

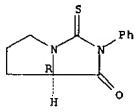
Absolute stereochemistry.



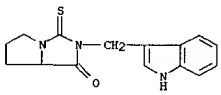
RN 175274-20-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 11 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



IT **175088-28-5**
RL: ANT (Analyte); PEP (Physical, engineering or chemical process); ANST (Analytical study); PROC (Process)
(reversed phase planar chromatog. on microcryst. triacetyl cellulose)
RN 175088-28-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-(1H-indol-3-ylmethyl)-3-thioxo- (9CI) (CA INDEX NAME)



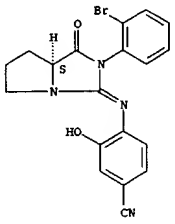
L12 ANSWER 12 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 2000:861490 CAPLUS
DOCUMENT NUMBER: 134:25357
TITLE: Phenyl urea IL-8 receptor antagonists for therapeutic use
INVENTOR(S): Palovich, Michael R.; Widdowson, Katherine L.
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 39 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000072845	A1	20001207	WO 2000-US14661	20000526

W: AE, AL, AU, BA, BB, BG, BR, CA, CN, CZ, DZ, EE, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, MZ, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, TZ, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
PRIORITY APPLN. INFO.: US 1999-136717 P 19990528
OTHER SOURCE(S): MARPAT 134:25357
AB The invention discloses the use of Ph ureas in the treatment of disease states mediated by the chemokine, Interleukin-8 (IL-8). Prepn. of compds. of the invention is described.
IT **311319-99-0P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(phenylurea IL-8 receptor antagonists for therapeutic use)
RN 311319-99-0 CAPLUS
CN Benzonitrile, 4-[[(7aS)-2-(2-bromophenyl)hexahydro-1-oxo-3H-pyrrolo[1,2-c]imidazol-3-ylidene]amino]-3-hydroxy- (9CI) (CA INDEX NAME)

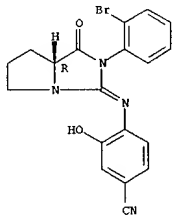
Absolute stereochemistry.
Double bond geometry unknown.

L12 ANSWER 12 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



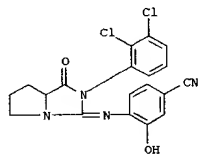
IT **311320-02-2 311320-03-3 311320-04-4**
311320-05-5 311320-06-6
RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(phenylurea IL-8 receptor antagonists for therapeutic use)
RN 311320-02-2 CAPLUS
CN Benzonitrile,
4-[[(7aR)-2-(2-bromophenyl)hexahydro-1-oxo-3H-pyrrolo[1,2-c]imidazol-3-ylidene]amino]-3-hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

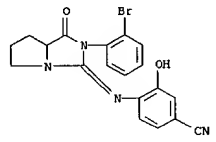


RN 311320-03-3 CAPLUS
CN Benzonitrile, 4-[[(7aS)-2-(2,3-dichlorophenyl)hexahydro-1-oxo-3H-pyrrolo[1,2-c]imidazol-3-ylidene]amino]-3-hydroxy- (9CI) (CA INDEX NAME)

L12 ANSWER 12 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
CN Benzonitrile,
4-[[2-(2,3-dichlorophenyl)hexahydro-1-oxo-3H-pyrrolo[1,2-c]imidazol-3-ylidene]amino]-3-hydroxy- (9CI) (CA INDEX NAME)



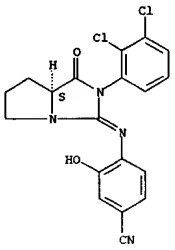
RN 311320-06-6 CAPLUS
CN Benzonitrile, 4-[[2-(2-bromophenyl)hexahydro-1-oxo-3H-pyrrolo[1,2-c]imidazol-3-ylidene]amino]-3-hydroxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1
REFERENCE(S): (1) Smithkline Beecham Corporation; WO 0035442 A1 2000
CAPLUS

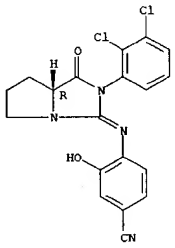
L12 ANSWER 12 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

Absolute stereochemistry.
Double bond geometry unknown.



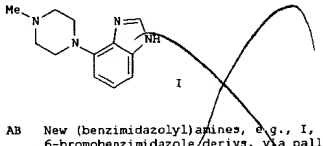
RN 311320-04-4 CAPLUS
CN Benzonitrile, 4-[[(7aR)-2-(2,3-dichlorophenyl)hexahydro-1-oxo-3H-pyrrolo[1,2-c]imidazol-3-ylidene]amino]-3-hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



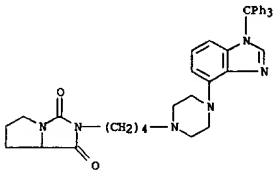
RN 311320-05-5 CAPLUS

L12 ANSWER 13 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 2000:359128 CAPLUS
DOCUMENT NUMBER: 133:120273
TITLE: Pd(0) amination of benzimidazoles as an efficient method towards new (benzimidazolyl)piperazines with high affinity for the 5-HT1A receptor
AUTHOR(S): Lopez-Rodriguez, Maria L.; Benhamu, Bellinda; Ayala, David; Rominguera, J. Luis; Murcia, Marta; Ramos, Jose A.; Viso, Alma
CORPORATE SOURCE: Departamento de Quimica Organica I, Facultad de Ciencias Quimicas, Universidad Complutense, Madrid, E-28040, Spain
SOURCE: Tetrahedron (2000), 56(20), 3245-3253
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:120273
GI

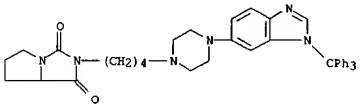


AB New (benzimidazolyl)amines, e.g., I, have been synthesized from 4- and 6-bromobenzimidazole derivs. via palladium-mediated amination reactions.
Among them, (benzimidazol-4(7)-yl)piperazine derivs. have been shown to be a new family of high affinity 5-HT1A receptor ligands.
IT **247083-16-5P 247083-17-6P**
RL: BAC (Biological activity or effector, except adverse); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(palladium-catalyzed amination of benzimidazoles and 5-HT1A receptor affinity of benzimidazolylpiperazines)
RN 247083-16-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-[4-[1-(triphenylmethyl)-1H-benzimidazol-4-yl]-1-piperazinyl]butyl]- (9CI) (CA INDEX NAME)

L12 ANSWER 13 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



RN 247083-17-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-[4-[1-(triphenylmethyl)-1H-benzimidazol-6-yl]-1-piperazinyl]butyl]- (9CI) (CA INDEX NAME)



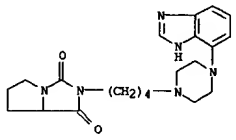
IT **247083-18-7P 247083-19-8P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(palladium-catalyzed amination of benzimidazoles and 5-HT1A receptor affinity of benzimidazolylpiperazines)
RN 247083-18-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[4-[4-(1H-benzimidazol-4-yl)-1-piperazinyl]butyl]tetrahydro- (9CI) (CA INDEX NAME)

L12 ANSWER 13 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

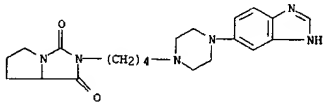
(5) Cheng, Y; Biochem Pharmacol 1973, V22, P3099 CAPLUS
(6) Clark, R; J Med Chem 1990, V33, P633 CAPLUS
(7) Edlin, C; Tetrahedron Lett 1998, V39, P2797 CAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

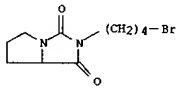
L12 ANSWER 13 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



RN 247083-19-8 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[4-[4-(1H-benzimidazol-5-yl)-1-piperazinyl]butyl]tetrahydro- (9CI) (CA INDEX NAME)

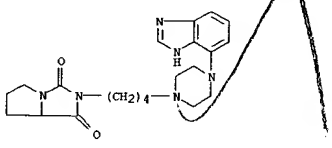


IT **181948-88-9**
RL: RCT (Reactant)
(palladium-catalyzed amination of benzimidazoles and 5-HT1A receptor affinity of benzimidazolylpiperazines)
RN 181948-88-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(4-bromobutyl)tetrahydro- (9CI) (CA INDEX NAME)



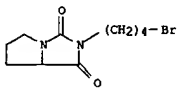
REFERENCE COUNT: 53
REFERENCE(S): (2) Belfield, A; Tetrahedron 1999, V55, P11399 CAPLUS
(3) Blettner, C; Synlett 1999, P307 CAPLUS

L12 ANSWER 14 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1999:571282 CAPLUS
DOCUMENT NUMBER: 131:299429
TITLE: Synthesis of new (benzimidazolyl)piperazines with affinity for the 5-HT1A receptor via Pd(0) amination of bromobenzimidazoles
AUTHOR(S): Lopez-Rodriguez, Maria L.; Viso, Alma; Benhamu, Bellinda; Rominguera, J. Luis; Murcia, Marta
CORPORATE SOURCE: Departamento de Quimica Organica I, Facultad de Ciencias Quimicas, Universidad Complutense, Madrid, E-28040, Spain
SOURCE: Bioorg. Med. Chem. Lett. (1999), 9(16), 2339-2342
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The synthesis of a new family of (benzimidazolyl)piperazines has been developed through Pd(0) mediated amination of 4- and 6-bromobenzimidazole derivs. Preliminary studies showed that some of these compds. are potent 5-HT1A receptor ligands.
IT **247083-18-7P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of benzimidazolylpiperazines with affinity for 5-HT1A receptor)
RN 247083-18-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[4-[4-(1H-benzimidazol-4-yl)-1-piperazinyl]butyl]tetrahydro- (9CI) (CA INDEX NAME)

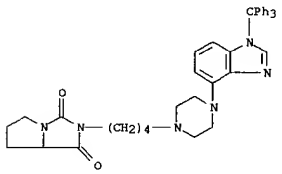


IT **181948-88-9**
RL: RCT (Reactant)
(prepn. of benzimidazolylpiperazines with affinity for 5-HT1A receptor)
RN 181948-88-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(4-bromobutyl)tetrahydro- (9CI) (CA INDEX NAME)

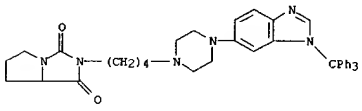
L12 ANSWER 14 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



IT **247083-16-5P 247083-17-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of benzimidazolylpiperazines with affinity for 5-HT1A receptor)
RN 247083-16-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-[4-[1-(triphenylmethyl)-1H-benzimidazol-4-yl]-1-piperazinyl]butyl]- (9CI) (CA INDEX NAME)

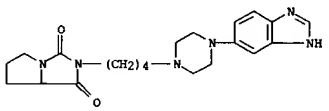


RN 247083-17-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-[4-[1-(triphenylmethyl)-1H-benzimidazol-6-yl]-1-piperazinyl]butyl]- (9CI) (CA INDEX NAME)



L12 ANSWER 14 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

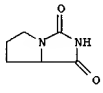
IT **247083-19-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of benzimidazolylpiperazines with affinity for 5-HT1A receptor)
RN 247083-19-8 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[4-[4-(1H-benzimidazol-5-yl)-1-piperazinyl]butyl]tetrahydro- (9CI) (CA INDEX NAME)



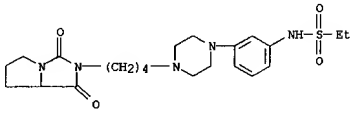
REFERENCE COUNT: 47
REFERENCE(S):
(3) Anon; GB 2097790 1983 CAPLUS
(5) Blettner, C; Synlett 1999, P307 CAPLUS
(7) Clark, R; J Med Chem 1990, V33, P633 CAPLUS
(8) Dandegaonker, S; J Karnatak Univ 1961, V6 CAPLUS
(9) Edlin, C; Tetrahedron Lett 1998, V39 CAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 15 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1999:404104 CAPLUS
DOCUMENT NUMBER: 131:179303
TITLE: Design and synthesis of 2-[4-[4-(m-(ethylsulfonamido)-phenyl)piperazin-1-YL]butyl]-1,3-dioxoperhydropyrrolo[1,2-c]imidazole (EF-7412) using neural networks. A selective derivative with mixed 5-HT1A/D2 antagonist properties
AUTHOR(S): Lopez-Rodriguez, Maria L.; Morcillo, M. Jose; Fernandez, Esther; Rosado, M. Luisa; Orensanz, Luis; Beneytez, M. Eugenia; Manzanares, Jorge; Fuentes, Jose A.; Schaper, Klaus-Jurgen
CORPORATE SOURCE: Departamento de Quimica Organica I, Facultad de Ciencias Quimicas, Universidad Complutense, Madrid, 28040, Spain
SOURCE: Bioorg. Med. Chem. Lett. (1999), 9(12), 1679-1682
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A test series of 32 phenylpiperazines with affinity for 5-HT1A and .alpha.1 receptors was subjected to QSAR anal. using artificial neural networks (ANNs), in order to get insight into the structural requirements that are responsible for 5-HT1A/.alpha.1 selectivity. Good models and predictive power were obtained for 5-HT1A and .alpha.1 receptors. A comparison of these models gives information for the design of the new ligand EF-7412 (5-HT1A:Ki (nM)=27; .alpha.1:Ki (nM) > 1000). This deriv. displayed affinity for dopamine D2 receptor (Ki=22 nM) and is selective for all other receptors examd. (5-HT2A, 5-HT3, 5-HT4 and Bz). EF-7412 acts as antagonist in vivo in pre- and postsynaptic 5-HT1A receptor sites and as an antagonist in dopamine D2 receptor.
IT **5768-79-6 221452-76-2**, EF 7412
RL: RCT (Reactant)
(design and synthesis of EF-7412 with mixed 5-HT1A/D2 antagonist properties)
RN 5768-79-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro- (9CI) (CA INDEX NAME)

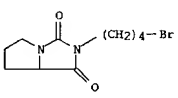
L12 ANSWER 15 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



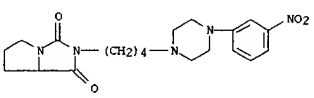
RN 221452-76-2 CAPLUS
CN Ethanesulfonamide, N-[3-[4-[4-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)butyl]-1-piperazinyl]phenyl]- (9CI) (CA INDEX NAME)



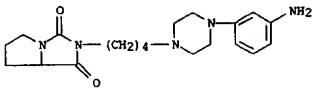
IT **181948-88-9P 188915-12-0P 188915-13-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(design and synthesis of EF-7412 with mixed 5-HT1A/D2 antagonist properties)
RN 181948-88-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(4-bromobutyl)tetrahydro- (9CI) (CA INDEX NAME)



RN 188915-12-0 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-[4-(3-nitrophenyl)-1-piperazinyl]butyl]- (9CI) (CA INDEX NAME)

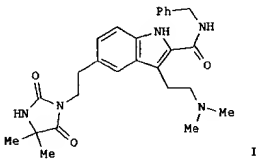


L12 ANSWER 15 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
RN 188915-13-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[4-[4-(3-aminophenyl)-1-piperazinyl]butyl]tetrahydro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12
REFERENCE(S):
(4) Gerhardt, C; Eur J Pharmacol 1997, V334, P1
CAPLUS
(5) Lopez-Rodriguez, M; Bioorg Med Chem Lett 1996, V6, P689 CAPLUS
(6) Lopez-Rodriguez, M; Bioorg Med Chem Lett 1998, V8, P581 CAPLUS
(7) Lopez-Rodriguez, M; J Med Chem 1996, V39, P4439 CAPLUS
(8) Lopez-Rodriguez, M; J Med Chem 1997, V40, P1648 CAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 16 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1999:377060 CAPLUS
DOCUMENT NUMBER: 131:170303
TITLE: Synthesis and Serotonergic Activity of Substituted 2-(N-Benzylcarboxamido)-5-[2-(2,5-dioxo-1-imidazolidinyl)ethyl]-N,N-dimethyltryptamine Derivatives: Novel Antagonists for the Vascular 5-HT1B-like Receptor
AUTHOR(S): Moloney, Gerard P.; Martin, Graeme R.; Mathews, Neil; Milne, Aynsley; Hobbs, Heather; Dodsworth, Susan; Sang, Pang Yih; Knight, Cameron; Williams, Marnie; Maxwell, Miles; Glen, Robert C.
CORPORATE SOURCE: Department of Medicinal Chemistry Victorian College of Pharmacy, Monash University, Parkville, 3052, Australia
SOURCE: J. Med. Chem. (1999), 42(14), 2504-2526
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

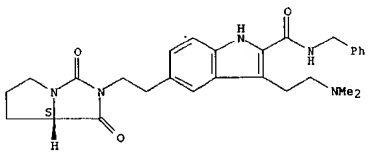


I

AB The synthesis and vascular 5-HT1B-like receptor activity of a novel series of substituted 2-(N-benzylcarboxamido)-5-[2-(2,5-dioxo-1-imidazolidinyl)ethyl]-N,N-dimethyltryptamine derivs., e.g. I, are described. Modifications to the 5-ethylene-linked heterocycle and to substituents on the 2-benzylamide side chain have been explored. Several compds. were identified which exhibited affinity at the vascular 5-HT1B-like receptor of pKB > 7.0, up to 100-fold selectivity over .alpha.1-adrenoceptor affinity and 5-HT2A receptor affinity, and which exhibited a favorable pharmacokinetic profile. I was identified as a highly potent, silent, and competitive vascular 5-HT1B-like receptor antagonist with a plasma elimination half-life of .apprx.4 h in dog plasma

L12 ANSWER 16 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
and with good oral bioavailability. The selectivity of compds. from this series for the vascular 5-HT1B-like receptors over other receptor subtypes is discussed as well as a proposed mode of binding to the receptor pharmacophore. It has been proposed that the arom. ring of the 2,N-benzylcarboxamide group can occupy an arom. binding site rather than the indole ring. The resulting conformation allows an amine-binding site to be occupied by the ethylamine nitrogen and a hydrogen-bonding site to be occupied by one of the hydantoin carbonyls. The electronic nature of the 2,N-benzylcarboxamide arom. group as well as the size of substituents on this arom. group is crucial for producing potent and selective antagonists. The structural requirement on the 3-ethylamine side chain incorporating the protonatable nitrogen is achieved by the bulky 2,N-benzylcarboxamide group and its close proximity to the 3-side chain.
IT **238427-88-8P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of N-benzylcarboxamido[(dioxoimidazolidinyl)ethyl]-N,N-dimethyltryptamines as serotonergic antagonist)
RN 238427-88-8 CAPLUS
CN 1H-Indole-2-carboxamide, 3-[2-(dimethylamino)ethyl]-N-(phenylmethyl)-5-[2-[(7aS)-tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl]ethyl]- (9CI) (CA INDEX NAME)

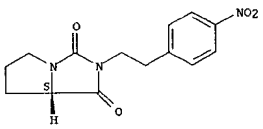
Absolute stereochemistry.



IT **238427-84-4P 238427-85-5P 238427-86-6P 238427-87-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of N-benzylcarboxamido[(dioxoimidazolidinyl)ethyl]-N,N-dimethyltryptamines as serotonergic antagonist)

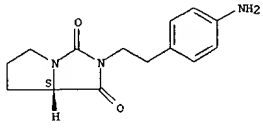
L12 ANSWER 16 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
RN 238427-84-4 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[2-(4-nitrophenyl)ethyl]-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 238427-85-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[2-(4-aminophenyl)ethyl]tetrahydro-, (7aS)- (9CI) (CA INDEX NAME)

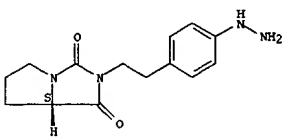
Absolute stereochemistry.



RN 238427-86-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[2-(4-hydrazinophenyl)ethyl]tetrahydro-, monohydrochloride, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

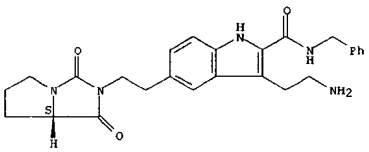
L12 ANSWER 16 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



● HCl

RN 238427-87-7 CAPLUS
CN 1H-Indole-2-carboxamide, 3-(2-aminoethyl)-N-(phenylmethyl)-5-[2-[(7aS)-tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 45
REFERENCE(S):
(1) Anon; EP 0533266 A1 1992 CAPLUS
(2) Anon; EP 0533267 A1 1992 CAPLUS
(3) Anon; EP 0533268 A1 1992 CAPLUS
(4) Bradley, P; Neuropharmacology 1986, V25, P563 CAPLUS
(5) Brieskorn, C; Arch Pharm 1978, V311, P954 CAPLUS

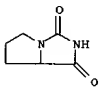
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 17 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1999:222937 CAPLUS
DOCUMENT NUMBER: 130:252384
TITLE: Process for preparing 2-[4-[4-(m-ethylsulfonamidophenyl)piperazin-1-yl]butyl]-1,3-dioxoperhydropyrrolo[1,2-c]imidazole
INVENTOR(S): Lopez Rodriguez, Maria Luz; Morcillo Ortega, Maria Jose; Fernandez Velando, Esther
PATENT ASSIGNEE(S): Universidad Complutense De Madrid, Spain
SOURCE: PCT Int. Appl., 15 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Spanish
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9915527	A1	19990401	WO 1998-ES250	19980915
W: AU, CA, JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
ES 2129370	A1	19990601	ES 1997-1987	19970923
ES 2129370	B1	20000301		
AU 9890730	A1	19990412	AU 1998-90730	19980915
PRIORITY APPLN. INFO.:			ES 1997-1987	19970923
			WO 1998-ES250	19980915

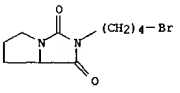
AB The title compd. (EF-7412), which is a 5-HT1A receptor antagonist, is prepd. by treating perhydropyrrolo[1,2-c]imidazole-1,3-dione with 1,4-dibromobutane, treating the 4-bromobutyl deriv. with 1-(3-nitrophenyl)piperazine, reducing the nitro group and ethanesulfonylating the amino group.

IT **5768-79-6**
RL: RCT (Reactant)
(prepn. of ethylsulfonamidophenylpiperazinylbutylperhydropyrroloimidazoledione EF-7412)
RN 5768-79-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro- (9CI) (CA INDEX NAME)

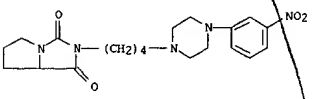


IT **181948-88-9P 188915-12-0P 188915-13-1P**

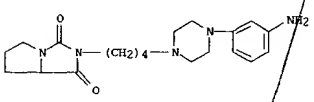
L12 ANSWER 17 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of ethylsulfonamidophenylpiperazinylbutylperhydropyrroloimidazoledione EF-7412)
RN 181948-88-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(4-bromobutyl)tetrahydro- (9CI) (CA INDEX NAME)



RN 188915-12-0 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-[4-(3-nitrophenyl)-1-piperazinyl]butyl]- (9CI) (CA INDEX NAME)

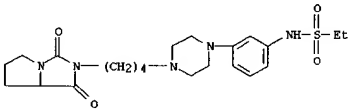


RN 188915-13-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[4-[4-(3-aminophenyl)-1-piperazinyl]butyl]tetrahydro- (9CI) (CA INDEX NAME)



IT **221452-76-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of ethylsulfonamidophenylpiperazinylbutylperhydropyrroloimidazoledione EF-7412)
RN 221452-76-2 CAPLUS
CN Ethanesulfonamide, N-[3-[4-[4-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)butyl]-1-piperazinyl]phenyl]- (9CI) (CA INDEX NAME)

L12 ANSWER 17 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



REFERENCE COUNT: 3
REFERENCE(S):
(1) Lopez-Rodriguez, M; Journal Medicinal Chemistry 1996, V39, P4439 CAPLUS
(2) Martin, G; Journal Medicinal Chemistry 1989, V32, P1052 CAPLUS
(3) Universidad Complutense de Madrid; WO 9606846 A 1996 CAPLUS

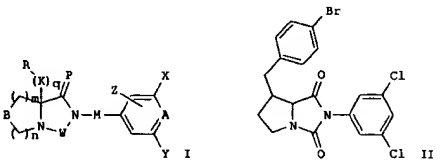
L12 ANSWER 18 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 2001:319894 CAPLUS
DOCUMENT NUMBER: 134:326532
TITLE: Preparation of 3-(hetero)aryl-1,3-diazabicyclo[3.3.0]octane-2,4-diones and analogs as inhibitors of .alpha.1.beta.2 mediated cell adhesion
INVENTOR(S): Sircar, Ila; Furth, Paul; Teegarden, Bradley R.; Morningstar, Marshall; Smith, Nicholas; Griffith, Ronald C.
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan
SOURCE: PCT Int. Appl., 195 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001030781	A2	20010503	WO 2000-US29273	20001019

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 1999-160629 P 19991020
US 2000-209847 P 20000607
OTHER SOURCE(S): MARPAT 134:326532
GI

L12 ANSWER 18 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

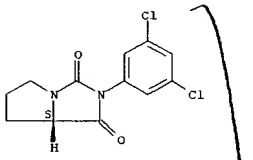


AB Title compds. (I) [wherein A = :CZ1 or :N; B = CH:CH, S, SO, SO2, O, or (un)substituted N or CH2; K = CH2, CHOH, CO, or CF2, M = a bond, (CH2)p, CO, or NH; W = CQ, CR6C(:Q), or C(:Q)CR6; X and Y = independently H, halo, NO2, CN, alkylthio, (halo)alkyl, alkoxy, acyl, or (un)substituted amino or (hetero)aryl; Z and Z1 = independently H, OH, halo, NO2, CF3, acyl, (un)substituted amino, carbamoyl, or alkoxy; P and Q = independently O or S; R = (un)substituted (hetero)aryl; R6 = H or (un)substituted alkyl; m = 0-3; n = 0-2; p and q = independently 1 or 2; or a pharmaceutically acceptable salt thereof] were prepd. as inhibitors of .alpha.1.beta.2 mediated cell adhesion. For example, 4-bromobenzyl bromide was added to N-(tert-butoxycarbonyl)proline Me ester in THF, the proline deprotected using TFA, 3,5-dichlorophenyl isocyanate added in the presence of DIEA in THF, and the dichlorophenylcarbamoyl deriv. cyclized using NaOEt in EtOH to afford II. In the Jurkat/ICAM-1 adhesion assay, I gave IC50 values from low nM to .mu.M. I are useful in the treatment of a variety of inflammatory diseases, including psoriasis, rheumatoid arthritis, inflammatory bowel diseases, systemic lupus erythematosus, atopic dermatitis, Sjogren's Syndrome, rejection after transplantation, and graft vs. host disease (no data).

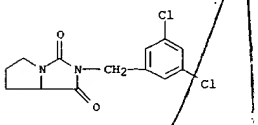
IT **336817-59-5P 336818-18-9P 336818-20-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(intermediate; prepn. of 3-(hetero)aryl-1,3-diazabicyclo[3.3.0]octane-2,4-diones and analogs as inhibitors of .alpha.1.beta.2 mediated cell adhesion by cyclization and reaction of N-[(hetero)arylcarbamoyl]prolin e derivs.)

RN 336817-59-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(3,5-dichlorophenyl)tetrahydro-, (7aS)- (9CI) (CA INDEX NAME)

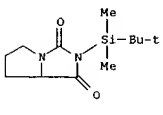
Absolute stereochemistry.



RN 336818-18-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[(3,5-dichlorophenyl)methyl]tetrahydro- (9CI) (CA INDEX NAME)

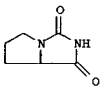


RN 336818-20-3 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[(1,1-dimethylethyl)dimethylsilyl]tetrahydro- (9CI) (CA INDEX NAME)



IT **5768-79-6**
RL: RCT (Reactant)
(starting material; prepn. of 3-(hetero)aryl-1,3-diazabicyclo[3.3.0]octane-2,4-diones and analogs as inhibitors of .alpha.1.beta.2 mediated cell adhesion by cyclization and reaction of N-[(hetero)arylcarbamoyl]proline derivs.)

RN 5768-79-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro- (9CI) (CA INDEX NAME)

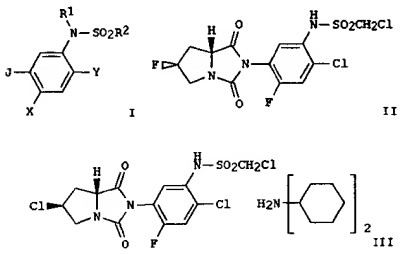


L12 ANSWER 19 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1997:390665 CAPLUS
DOCUMENT NUMBER: 127:17676
TITLE: Herbicidal N-(heterocyclylphenyl)sulfonamides as herbicides
INVENTOR(S): Adams, Edward John; Drauz, Karlheinz; Hong, Wonpyo; Kamireddy, Balreddy; Petersen, Wallace Christian; Schafer, Matthias; Weckbecker, Christoph; et al.
PATENT ASSIGNEE(S): E.I. Du Pont De Nemours and Company, USA; Adams, Edward John; Drauz, Karlheinz; Hong, Wonpyo
SOURCE: PCT Int. Appl., 314 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9715576	A1	19970501	WO 1996-US16111	19961008
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KG, KP, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9675153	A1	19970515	AU 1996-75153	19961008
AU 712362	B2	19991104		
EP 862571	A1	19980909	EP 1996-937667	19961008
R: AT, BE, DE, DK, ES, FR, GB, GR, IT, IE				
CN 1202172	A	19981216	CN 1996-197871	19961008
BR 9611133	A	19990525	BR 1996-11133	19961008
JP 11514370	T2	19991207	JP 1996-516120	19961008
US 6060432	A	20000509	US 1996-736636	19961024

PRIORITY APPLN. INFO.: US 1995-7031 P 19951025
US 1996-12329 P 19960227
WO 1996-US16111 W 19961008

OTHER SOURCE(S): MARPAT 127:17676
GI



L12 ANSWER 19 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

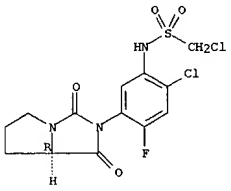
AB The title compds. [I; J = (un)substituted heterocyclyl, (un)substituted heterocyclylcarboxamido, (un)substituted heterocyclylideneimino, etc.; R1 = C1-6 alkyl, C1-6 haloalkyl, C3-6 alkenyl, etc.; R2 = C1-C6 alkoxy, C1-C6 haloalkoxy, C1-C6 haloalkyl, C3-C6 cycloalkyl, C3-C6 halocycloalkyl, C2-C6 alkoxyalkyl, C2-C6 haloalkoxyalkyl, C2-C6 alkenyl, C2-C6 haloalkenyl, C3-C6 alkoxyalkenyl, C2-C6 alkynyl, C2-C6 haloalkynyl, C2-C6 cyanoalkyl, C1-C6 nitroalkyl, (CH2)p-OR6, CH=CH(CH2)q-OR6, C.tplbond.C(CH2)q-OR6, C2-C6 alkylthioalkyl, C2-C6 alkylsulfinylalkyl, C2-C6 alkylsulfonylalkyl, C3-C8 alkoxycarbonylalkyl, C3-C8 alkylcarbonyloxyalkyl, or oxiranyl optionally substituted with 1-3 C1-C3 alkyl; R6 = C1-3 alkylsulfonyl, dialkoxyphosphinyl, (alkyl)phenylsulfonyl, etc.; X = H, F, Cl; Y = F, Cl, Br, cyano, nitro, C1-3 haloalkyl, etc.] and their N-oxides and agriculturally suitable salts are prepd. Thus, the title compd. II was prepd. in 8 steps from N-(4-chloro-2-fluorophenyl)acetamide, chloromethylsulfonyl chloride, phosgene, and 4-cis-D-hydroxyproline. III (also prepd.) at 2000 g/ha had a 100% kill against barnyard grass.

IT **190314-48-8P 190314-49-9P 190314-50-2P 190314-51-3P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); SFN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of herbicidal (heterocyclylphenyl)sulfonamides)

L12 ANSWER 19 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

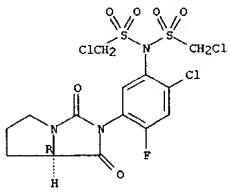
RN 190314-48-8 CAPLUS
CN Methanesulfonamide, 1-chloro-N-[2-chloro-4-fluoro-5-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)phenyl]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 190314-49-9 CAPLUS
CN Methanesulfonamide, 1-chloro-N-[2-chloro-4-fluoro-5-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)phenyl]-N-[(chloromethyl)sulfonyl]-, (R)- (9CI) (CA INDEX NAME)

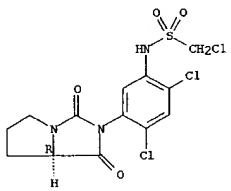
Absolute stereochemistry.



RN 190314-50-2 CAPLUS
CN Methanesulfonamide, 1-chloro-N-[2,4-dichloro-5-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)phenyl]-, (R)- (9CI) (CA INDEX NAME)

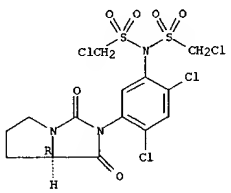
L12 ANSWER 19 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

Absolute stereochemistry.

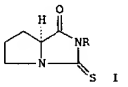


RN 190314-51-3 CAPLUS
CN Methanesulfonamide, 1-chloro-N-[(chloromethyl)sulfonyl]-N-[2,4-dichloro-5-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)phenyl]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 20 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1990:21262 CAPLUS
DOCUMENT NUMBER: 112:21262
TITLE: Proton magnetic resonance study of the conformation of the pyrrolidine ring in some proline-thiohydantoins
AUTHOR(S): Sleeckx, Jef J. M.; Anteunis, Marc J. O.; Borremans, Frans A. M.
CORPORATE SOURCE: Lab. Org. Chem., Rijksuniv. Gent., Ghent, B-9000, Belg.
SOURCE: Collect. Czech. Chem. Commun. (1988), 53(11A), 2503-10
CODEN: CCCCAK; ISSN: 0010-0765
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:21262
GI



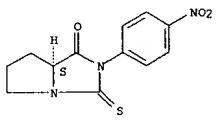
I

AB The conformational behavior of a series of N-substituted thiohydantoins I (R = H, Me, Ph, 4-O2NC6H4) of proline was studied by 1H NMR. The pseudorotational parameters of the proline moiety were calcd. from the ten vicinal proton-proton coupling consts. assuming a two state equil. (N .dblharw. S). The effect of the different substituents at the thiohydantoin N on the conformation of the pyrrolidine rings is discussed. The spectrum of I (R = Me) was recorded at different temps. in toluene-d8 solns. The conformational anal. of these spectra showed that the ratio of the populations of the N and S forms changes considerably with temp., while the conformational identity of both the N and S forms remains strictly preserved. These facts provide an addnl. exptl. justification of the two-state assumption, at least for the present model compds.

IT **61160-12-1**
RL: PRP (Properties)
(conformation of, by proton NMR, pseudorotation in)
RN 61160-12-1 CAPLUS

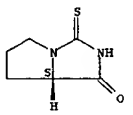
L12 ANSWER 20 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
(S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



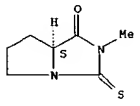
L12 ANSWER 20 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-3-thioxo-, (7aS)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.



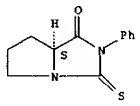
IT **28868-23-7P 29635-99-2P 124312-49-8P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conformation of, by proton NMR, pseudorotation in)
RN 28868-23-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo-, (7aS)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



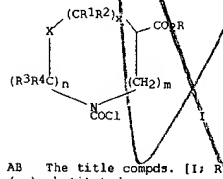
RN 124312-49-8 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one,
hexahydro-2-(4-nitrophenyl)-3-thioxo-,

=> d ibib abs hitstr 21-40

L12 ANSWER 21 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1983:438810 CAPLUS
DOCUMENT NUMBER: 99:38810
TITLE: N-Chlorocarbonyl amino acid esters and their use
INVENTOR(S): Drauz, Karlhein; Kleemann, Axel
PATENT ASSIGNEE(S): Degussa A.-G., Fed. Rep. Ger.
SOURCE: Eur. Pat. Appl., 27 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

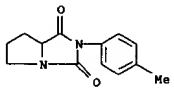
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 75737	A1	19830406	EP 1982-107925	19820828
R: AT, BE, CH, DE, FR, GB, IT, LI, NL				
DE 3137376	A1	19830505	DE 1981-3137376	19810919
DE 3137376	C2	19860227		
ES 515476	A1	19830601	ES 1982-515476	19820903
JP 58065266	A2	19830418	JP 1982-161063	19820917
JP 03041466	B4	19910624		
CA 1184177	A1	19850319	CA 1982-411699	19820917
JP 59093068	A2	19840529	JP 1983-169542	19830916

PRIORITY APPLN. INFO.: DE 1981-3137376 19810919
GI

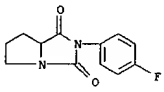


AB The title compds. [I; R = alkyl; R1-R3 = H, alkyl; R4 = H, (un)substituted alkyl, aryl, heteroaryl; R3R4 = alkylene; X = CH2, S; n, m, x = 0-2; n + m + x = 1-3] were prepd. Thus, L-proline Me ester HCl was treated with NH3 to prep. the free ester and phosgenated to give 93.5% 1-(chlorocarbonyl)-L-proline Me ester. I are intermediates in prepn. of plant protection agents.
IT **60725-55-5P 60725-58-8P 60725-61-3P 60725-79-3P**

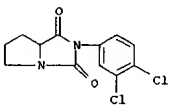
L12 ANSWER 21 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)
RN 60725-55-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-(4-methylphenyl)- (9CI) (CA INDEX NAME)



RN 60725-58-8 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(4-fluorophenyl)tetrahydro- (9CI) (CA INDEX NAME)

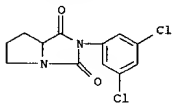


RN 60725-61-3 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(3,4-dichlorophenyl)tetrahydro- (9CI) (CA INDEX NAME)

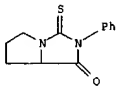


RN 60725-79-3 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(3,5-dichlorophenyl)tetrahydro- (9CI) (CA INDEX NAME)

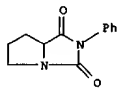
L12 ANSWER 21 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



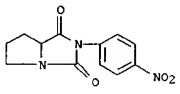
L12 ANSWER 22 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1983:416091 CAPLUS
DOCUMENT NUMBER: 99:16091
TITLE: Inhibition of .alpha.-chymotrypsin by 5-substituted-3-phenyl-2-thioxo-4-imidazolidinones and derivatives
AUTHOR(S): Mammo, Layla A.; Faden, Al. K.; Smith, H. J.; Sewell, R. D. E.
CORPORATE SOURCE: Welsh Sch. Pharm., Univ. Wales Inst. Sci. Technol., Cardiff, CF1 3NU, UK
SOURCE: J. Pharm. Pharmacol. (1982), 34(11), 752-4
CODEN: JPPMAB; ISSN: 0022-3573
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The inhibitory effects of phenylthiohydantoin (PTH)-amino acids (5-substituted-3-phenyl-2-thioxo-4-imidazolidinones) and derivs. on purified bovine pancreatic chymotrypsin [9004-07-3] were examd. and structure-activity relations were examd. The most active inhibitors were PTH-dehydroserine [85915-89-5] >> PTH-histidine [5835-68-7] > PTH-serine [5789-22-0]; PTH-arginine [4405-04-3], PTH-proline [**4333-21-5**], and PTH-hydroxyproline [85915-90-8] reduced the enzyme activity after several h to a const. level (approx.40% residual activity). Many of the PTH-amino acids were screened for analgesic activity, but only PTH-arginine, PTH-histidine, and PTH-hydroxyproline showed weak activity. These compds. were among the most potent PTH-amino acid inhibitors of chymotrypsin, which together with the analgesic activity data suggests that there may be a correlation between this property and the ability to acylate a nucleophilic group on a mol. participating directly or indirectly in the analgesic response.
IT **4333-21-5**
RL: BIOL (Biological study) (chymotrypsin inhibition by, structure and analgesic activity in relation to)
RN 4333-21-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo- (9CI) (CA INDEX NAME)



L12 ANSWER 22 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
IT **2221-09-2P 85915-88-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction with chymotrypsin)
RN 2221-09-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-phenyl- (9CI) (CA
INDEX NAME)

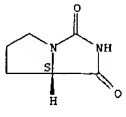


RN 85915-88-4 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione,
tetrahydro-2-(4-nitrophenyl)-
(9CI) (CA INDEX NAME)



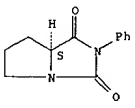
L12 ANSWER 23 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
RL: PRP (Properties)
(UV and CD spectrum of)
RN 40856-87-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-, (7aS)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.



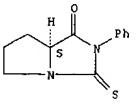
RN 70741-88-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-phenyl-, (7aS)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

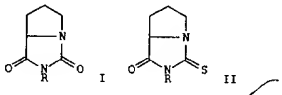


IT **29635-99-2**
RL: PRP (Properties)
(hindered rotation in)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-
(9CI) (CA INDEX NAME)

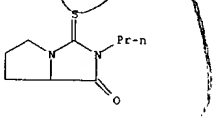
Absolute stereochemistry.



L12 ANSWER 23 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1979:438801 CAPLUS
DOCUMENT NUMBER: 91:38801
TITLE: CD spectroscopic evidence on the hindered rotation around the nitrogen-carbon bond in 3-phenyl-2-thiohydantoins
AUTHOR(S): Siemion, Ignacy Z.; Szkoda, Maria
CORPORATE SOURCE: Inst. Chem., Univ. Wroclaw, Wroclaw, 50-383, Pol.
SOURCE: Bull. Acad. Pol. Sci., Ser. Sci. Chim. (1978), 26(11), 851-7
CODEN: BAPCAQ; ISSN: 0001-4095
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

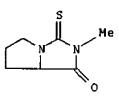


AB The UV and CD spectra of I (R = H, Ph) and of II (R = Ph, Pr) were detd.
In the case of 3-phenyl-2-thiohydantoin, the rotation about the N-Caryl
bond is hindered.
IT **70741-89-8**
RL: PRP (Properties)
(UV and CD spectra of)
RN 70741-89-8 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-propyl-3-thioxo- (9CI) (CA
INDEX NAME)



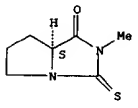
IT **40856-87-9 70741-88-7**

L12 ANSWER 24 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 2000:665309 CAPLUS
DOCUMENT NUMBER: 133:368875
TITLE: Enantiomer separation by capillary electrochromatography on a cyclodextrin-modified monolith
AUTHOR(S): Wistuba, Dorothee; Schurig, Volker
CORPORATE SOURCE: Institute of Organic Chemistry, University of Tubingen, Tubingen, 72076, Germany
SOURCE: Electrophoresis (2000), 21(15), 3152-3159
CODEN: ELCTIN; ISSN: 0173-0835
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A chiral monolithic stationary phase was prepd. by packing a capillary with bare porous silica and sintering the silica bed at high temp. The resulting silica monolith was polymer-coated with Chirasil-Dex, a permethylated .beta.-cyclodextrin covalently linked via an octamethylene spacer to dimethylpolysiloxane. Subsequently, Chirasil-Dex was thermally immobilized on the silica support and a chiral monolith of very high stability (30 kV, >400 bar pressure) was obtained. The enantiomer sepn. of various chiral compds. by monolithic (rod) capillary electrochromatog. (rod-CEC) was feasible. This method was compared with capillary liq. chromatog. (LC) in a single-column mode using unified equipment. About two to three times higher efficiency was found in the rod-CEC mode as compared to rod-LC. The influence of pressure-driven flow support on efficiency, resoln., elution time and baseline stability was studied. The amt. and nature of org. modifier strongly influences efficiency and resoln.
IT **22712-58-9 28868-23-7 145552-40-5**
RL: ANT (Analyte); PEP (Physical, engineering or chemical process); ANST
(Analytical study); PROC (Process)
(prepn. of cyclodextrin-modified monolith for capillary electrochromatog. resoln. of)
RN 22712-58-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo- (9CI) (CA
INDEX NAME)



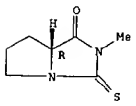
L12 ANSWER 24 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
RN 28868-23-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 145552-40-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo-, (7aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 51
REFERENCE(S):
(1) Armstrong, D; Anal Chem 1993, V65, P1114 CAPLUS
(2) Asiaie, R; J Chromatogr A 1998, V806, P251 CAPLUS
(3) Behnke, B; J Chromatogr A 1995, V716, P207 CAPLUS
(4) Carter-Finch, A; J Chromatogr A 1999, V848, P375 CAPLUS
(6) Dermaux, A; J High Resolut 1998, V21, P575 CAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

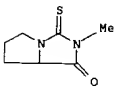
L12 ANSWER 25 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 2000:436780 CAPLUS
DOCUMENT NUMBER: 133:232148
TITLE: Enantiomer separation by complexation SFC on immobilized Chirasil-nickel and Chirasil-zinc selectands
AUTHOR(S): Schurig, V.; Fluck, M.
CORPORATE SOURCE: Institute of Organic Chemistry, University of Tubingen, Tubingen, 72076, Germany
SOURCE: J. Biochem. Biophys. Methods (2000), 43(1-3), 223-240
CODEN: JBBMDG; ISSN: 0165-022X
PUBLISHER: Elsevier Science Ireland Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The use of complexation SFC for enantiomer sepn. of Lewis base selectands on chiral nickel(II)- and zinc(II)-bis[(3-heptafluorobutanoyl)-10-methylene-(1R)-camphorate] chem. bonded to poly(dimethylsiloxane) (Chirasil-nickel and Chirasil-zinc) and employed as Lewis acid selectors is described. The method is esp. suited for less volatile and configurationally labile racemates. The variation of the exptl. parameters temp. T, pressure p and d. .rho. of the mobile phase carbon dioxide on the retention factor k, relative retention r and chiral sepn. factor .alpha. was studied, providing insights into the mechanisms of chiral recognition under supercrit. conditions. For mecoprop Me ester (Me 2-(4-chloro-2-methylphenoxy)propanoate) an unusual increase of .alpha. at increased temp. is obsd. on Chirasil-nickel. Supercrit. carbon dioxide does not inadvertently affect the complexation equil. between Lewis donor selectands and the Lewis acid metal selectors during complexation SFC.

IT 22712-58-9 28868-23-7 145552-40-5
RL: ANT (Analyte); PEP (Physical, engineering or chemical process); ANST (Analytical study); PROC (Process)
(enantiomer sepn. by complexation SFC on immobilized Chirasil-nickel and Chirasil-zinc)

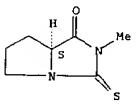
RN 22712-58-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo- (9CI) (CA INDEX NAME)

L12 ANSWER 25 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



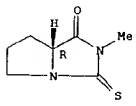
RN 28868-23-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 145552-40-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo-, (7aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



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REFERENCE(S):
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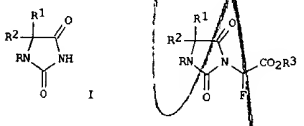
(4) Chester, T; J Microcol Sep 1993, V5, P127 CAPLUS
(6) Donnecke, J; J Microcol Sep 1996, V8, P495 CAPLUS
(7) Giddings, J; Anal Chem 1964, V36, P741 CAPLUS
(8) Giddings, J; Science 1968, V162, P67 CAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 26 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 2000:281658 CAPLUS
DOCUMENT NUMBER: 133:150868
TITLE: Synthesis of carbonyl-bridged peptides containing an .alpha.-fluoroglycine residue
AUTHOR(S): Takeuchi, Yoshio; Kirihara, Kiyotoshi; Shibata, Norio; Kirk, Kenneth L.
CORPORATE SOURCE: Fac. Pharm. Sci., Toyama Medical and Pharmaceutical University, Toyama, Japan
SOURCE: Chem. Commun. (Cambridge) (2000), (9), 785-786
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:150868
GI



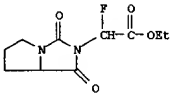
AB Gabriel reaction of hydantoins I (R = H, Boc; R1 = H, Me, Ph, iso-Pr, CH2Ph; R2 = H, Me, Ph, etc.) with BrFCHCO2R3 (R3 = Et, tert-Bu) provides a general method for the synthesis of carbonyl-bridged peptides II contg. an .alpha.-fluoroglycine residue.

IT 5768-79-6
RL: RCT (Reactant)
(prepn. of fluoroglycine-contg., carbonyl-bridged peptides via Gabriel reaction of hydantoins with bromofluoroacetates)

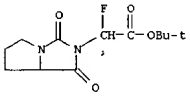
RN 5768-79-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro- (9CI) (CA INDEX NAME)

IT 287738-27-6P 287738-28-7P

L12 ANSWER 26 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of fluoroglycine-contg., carbonyl-bridged peptides via Gabriel
reaction of hydantoins with bromofluoroacetates)
RN 287738-27-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-2(3H)-acetic acid, .alpha.-fluorotetrahydro-1,3-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 287738-28-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-2(3H)-acetic acid, .alpha.-fluorotetrahydro-1,3-dioxo-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 11
REFERENCE(S):
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(3) Bailey, P; Tetrahedron Lett 1998, V39, P7755 CAPLUS
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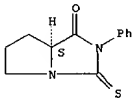
(9) Takeuchi, Y; Chem Pharm Bull 1998, V46, P1062 CAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 27 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

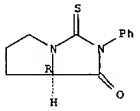
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 175274-20-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 13
REFERENCE(S):
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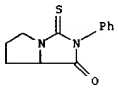
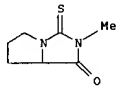
(6) Imai, K; Biomed Chromatogr 1995, V9, P195 CAPLUS
(7) Kim, B; J Liq Chrom & Related Technol 1999, V22, P523 CAPLUS
(8) Lee, W; Chromatographia 1999, V49, P61 CAPLUS
(9) Okamoto, Y; Chem Lett 1988, P1125 CAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 27 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 2000:100910 CAPLUS
DOCUMENT NUMBER: 132:216262
TITLE: Liquid chromatographic separation of the enantiomers of phenylthiohydantoin .alpha.-amino acids derivatives on polysaccharide-based chiral stationary phases
AUTHOR(S): Lee, Wonjae
CORPORATE SOURCE: LG Chemical Ltd., Taejon, 305-380, S. Korea
SOURCE: Anal. Lett. (2000), 33(2), 347-356
CODEN: ANALBP; ISSN: 0003-2719
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The liq. chromatog. enantiosepn. of the phenylthiohydantoin (PTH) derivs. of various amino acids on four com. polysaccharide-derived chiral stationary phases (CSPs) is described. Chiralcel OF and Chiralpak AS showed better performance than the other CSPs for resoln. of the enantiomers of PTH amino acid derivs. The enantiomers of all amino acids as their PTH derivs. were well sepd. on Chiralcel OF and/or Chiralpak AS. The (-)(L) or (-)-enantiomers of all analytes examd. were preferentially retained on Chiralpak AS, whereas the (+)(D) or (+)-enantiomers of most of analytes were preferentially retained on Chiralcel OF.
IT 4333-21-5, Phenylthiohydantoin DL-proline 29635-99-2, Phenylthiohydantoin L-proline 175274-20-1, Phenylthiohydantoin D-proline
RL: ANT (Analyte); PEP (Physical, engineering or chemical process); PRP (Properties); ANST (Analytical study); PROC (Process)
(liq. chromatog. sepn. of enantiomers of phenylthiohydantoin .alpha.-amino acids derivs. on polysaccharide-based chiral stationary phases)
RN 4333-21-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo- (9CI) (CA INDEX NAME)

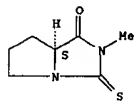


L12 ANSWER 28 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1999:675014 CAPLUS
DOCUMENT NUMBER: 131:331555
TITLE: Enantiomer separation by pressure-supported electrochromatography using capillaries packed with Chirasil-Dex polymer-coated silica
AUTHOR(S): Wistuba, Dorothee; Schurig, Volker
CORPORATE SOURCE: Institut fur Organische Chemie, Universitat Tubingen, Tubingen, D-72076, Germany
SOURCE: Electrophoresis (1999), 20(13), 2779-2785
CODEN: ELCTDN; ISSN: 0173-0835
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Pressure-supported electrochromatog. using capillaries packed with permethylcyclodextrin covalently linked via an octamethylene spacer to dimethylpolysiloxane and immobilized on silica (Chirasil-Dex silica) was employed as an efficient and rapid method for the enantiomer sepn. of various racemic compds. By comparing this method with micropacked liq. chromatog. (LC), employing the same column in a unified instrumental setup, micropacked capillary electrochromatog. (CEC) shows higher column efficiencies and hence better resoln. factors. The influence of type and concn. of buffer, amt. and nature of org. modifier, and pressure support was studied.
IT 22712-58-9, MTH-DL-proline 28868-23-7, MTH-L-proline 145552-40-5, MTH-D-proline
RL: ANT (Analyte); PEP (Physical, engineering or chemical process); ANST (Analytical study); PROC (Process)
(enantiomer sepn. by pressure-supported electrochromatog. using capillaries packed with Chirasil-Dex polymer-coated silica)
RN 22712-58-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo- (9CI) (CA INDEX NAME)



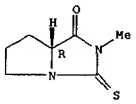
RN 28868-23-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

L12 ANSWER 28 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
Absolute stereochemistry.



RN 145552-40-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo-, (7aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 30
REFERENCE(S):
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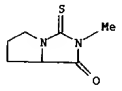
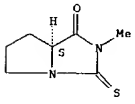
(2) Behnke, B; J Chromatogr A 1995, V716, P207 CAPLUS
(4) Deng, Y; Anal Chem 1998, V70, P4586 CAPLUS
(5) Dermaux, A; J High Res Chromatogr 1998, V21, P575 CAPLUS
(6) Francotte, E; Chromatographia 1996, V42, P521 CAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 29 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1998:478479 CAPLUS
DOCUMENT NUMBER: 129:197341
TITLE: Enantiomer separation by pressure-supported electrochromatography using capillaries packed with a permethyl-.beta.-cyclodextrin stationary phase
AUTHOR(S): Wistuba, D.; Czesla, H.; Roeder, M.; Schurig, V.
CORPORATE SOURCE: Institute of Organic Chemistry, University of Tubingen, Auf der Morgenstelle 18, Tubingen, D-72076, Germany
SOURCE: J. Chromatogr., A (1998), 815(2), 183-188
CODEN: JCRAEY; ISSN: 0021-9673
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Efficient enantiomer sepn. by pressure-assisted, micro-packed capillary electrochromatog. (CEC) was carried out using a permethyl-.beta.-cyclodextrin-modified silica support (PM-.beta.-CD-silica). When comparing this method with micro-packed-HPLC in the single-column-mode, CEC displays higher column efficiencies (about three times higher theor. plate nos. at comparable elution times). The pressure support (.apprx.10 bar), applied to avoid bubble formation, has a negligible influence on elution times in CEC. The influence and compn. of org. modifiers is described.
IT 22712-58-9 28868-23-7 145552-40-5
RL: ANT (Analyte); PEP (Physical, engineering or chemical process); ANST (Analytical study); PROC (Process)
(enantiomer sepn. by pressure-supported electrochromatog. using capillaries packed with permethyl-.beta.-cyclodextrin modified silica stationary phase)
RN 22712-58-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo- (9CI) (CA INDEX NAME)



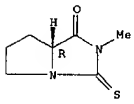
L12 ANSWER 29 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
RN 28868-23-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

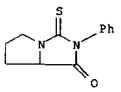


RN 145552-40-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo-, (7aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



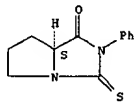
L12 ANSWER 30 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1998:353140 CAPLUS
DOCUMENT NUMBER: 129:89635
TITLE: Optical resolution ability of optically active poly(N-diphenylmethyl maleimide)
AUTHOR(S): Liu, Weihong; Shao, Lianhe; Chen, Yongming; Chen, Chuanfu; Liu, Guoquan; Xi, Fu
CORPORATE SOURCE: Institute Chem., Chinese Academy Sciences, Beijing, 100080, Peop. Rep. China
SOURCE: Chin. Sci. Bull. (1998), 43(3), 220-223
CODEN: CSBUEF; ISSN: 1001-6538
PUBLISHER: Science in China Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A new optically active polymer, (+)-poly(N-diphenylmethyl maleimide), was coated on macroporous silica gel and used as a chiral stationary phase for HPLC resoln. of enantiomers. The chiral polymer showed efficient resoln. ability to some polar racemates, and eleven pairs of racemates are resolved effectively.
IT 4333-21-5 29635-99-2 175274-20-1
RL: ANT (Analyte); PEP (Physical, engineering or chemical process); ANST (Analytical study); PROC (Process)
(active poly(N-diphenylmethyl maleimide) coated silica gel packing for HPLC enantiomer resoln. of)
RN 4333-21-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo- (9CI) (CA INDEX NAME)



RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

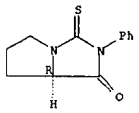
Absolute stereochemistry.

L12 ANSWER 30 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



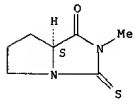
RN 175274-20-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



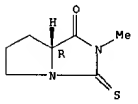
L12 ANSWER 31 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

Absolute stereochemistry.

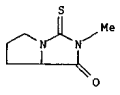


RN 145552-40-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo-, (7aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



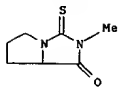
L12 ANSWER 31 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1997:211831 CAPLUS
DOCUMENT NUMBER: 126:338170
TITLE: Enantioselective capillary gas chromatography and capillary supercritical fluid chromatography on an immobilized .gamma.-cyclodextrin derivative
AUTHOR(S): Grosenick, Heiko; Schurig, Volker
CORPORATE SOURCE: Inst. Organische Chemie, Univ. Tubingen, Tubingen, D-72076, Germany
SOURCE: J. Chromatogr., A (1997), 761(1 + 2), 181-193
CODEN: JCRAEY; ISSN: 0021-9673
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Octakis(3-O-butanoyl-2,6-di-O-n-pentyl)-.gamma.-cyclodextrin (3-bu-2,6-pe-.gamma.-CD) was chem. linked to a polysiloxane via an octamethylene spacer, yielding a chiral stationary phase called Chirasil-.gamma.-Dex. Its immobilization onto the surface of capillary columns is possible by thermal treatment. The influence of the percentage of 3-bu-2,6-pe-.gamma.-CD in the stationary phase was systematically studied. With an increasing percentage of cyclodextrin, chiral sepn. factors, .alpha., and retention factors, k', increased, whereas the degree of immobilization decreased. A value of 40% (wt./wt.) 3-bu-2,6-pe-.gamma.-CD is optimal, since high sepn. factors are combined with a good degree of immobilization. Besides applications in enantioselective gas chromatog., some enantiomer sepns. by capillary supercrit. fluid chromatog. are presented.
IT **22712-58-9 28868-23-7 145552-40-5**
RL: ANT (Analyte); ANST (Analytical study)
(enantiomer sepn. by capillary supercrit. fluid chromatog. using immobilized Chirasil-.gamma.-Dex as chiral stationary phase)
RN 22712-58-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo- (9CI) (CA INDEX NAME)



RN 28868-23-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

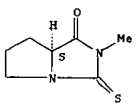
L12 ANSWER 32 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1997:58029 CAPLUS
DOCUMENT NUMBER: 126:220124
TITLE: The enantioresolution of methylthiohydantoin-amino acids on R,S-2-hydroxypropyl derivatized .beta.-cyclodextrin bonded stationary phase using the water-based mobile phase
AUTHOR(S): Chen, Shushi
CORPORATE SOURCE: Department of Food Nutrition, China Junior College of Medical Technology, Jen-Te, 70705, Taiwan
SOURCE: J. Chin. Chem. Soc. (Taipei) (1996), 43(6), 503-506
CODEN: JCCTAC; ISSN: 0009-4536
PUBLISHER: Chinese Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The HPLC enantioresoln. of thirteen methylthiohydantoin-amino acids (MTH-amino acids), which are substrates for producing D-amino acids through enzyme-catalyzed hydrolysis, is described on R,S-2-hydroxypropyl derivatized .beta.-cyclodextrin bonded stationary phase (RSP-.beta.-CD CSP) with a H2O-based mobile phase. The enantioresoln. is relatively sensitive to the structural variation of group which is attached to the C at position five on methylthiohydantoin moiety and subsequently turns into side-chain group of corresponding D-amino acid produced after hydrolysis. The inclusion complexation is believed to be the mechanism responsible for the obsd. enantioresoln. that cannot be reproduced either on native .beta.-cyclodextrin CSP under the same chromatog. conditions or on both CSPs using the MeCN-based mobile phase. Approaches for enantioimprovement include varying the percentage of org. modifier in the mobile phase and using the buffer-typed mobile phase such as triethylammonium acetate (pH 4.1).
IT **22712-58-9 28868-23-7 145552-40-5**
RL: ANT (Analyte); PEP (Physical, engineering or chemical process); ANST (Analytical study); PROC (Process)
(HPLC enantioresoln. of methylthiohydantoin-amino acids on R,S-2-hydroxypropyl derivatized .beta.-cyclodextrin bonded stationary phase using the water-based mobile phase)
RN 22712-58-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo- (9CI) (CA INDEX NAME)

L12 ANSWER 32 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



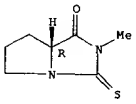
RN 28868-23-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

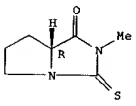


RN 145552-40-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo-, (7aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

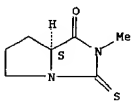


L12 ANSWER 33 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



L12 ANSWER 33 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1996:750759 CAPLUS
DOCUMENT NUMBER: 126:112546
TITLE: Enantiomer separation on a Chirasil-Dex-polymer-coated stationary phase by conventional and micro-packed high-performance liquid chromatography
AUTHOR(S): Schurig, V.; Negura, S.; Mayer, S.; Reich, S.
CORPORATE SOURCE: Institut fuer Organische Chemie, Universitaet Tuebingen, Auf der Morgenstelle 18, 72076, Tubingen, Germany
SOURCE: J. Chromatogr., A (1996), 755(2), 299-307
CODEN: JCRAEY; ISSN: 0021-9673
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Polymer-coating of Chirasil-Dex (a polysiloxane-anchored permethyl-.beta.-cyclodextrin) on Nucleosil 300-5 followed by thermal immobilization furnishes a chiral stationary phase for enantiomer sepn. under reversed-phase conditions by conventional and micro-packed HPLC.
IT **1968-34-9 28868-23-7 145552-40-5**
RL: ANT (Analyte); ANST (Analytical study)
(enantiomer sepn. by HPLC using Chirasil-Dex-polymer-coated chiral stationary phase)
RN 1968-34-9 CAPLUS
RN 28868-23-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



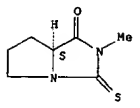
RN 145552-40-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo-, (7aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 34 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1993:72825 CAPLUS
DOCUMENT NUMBER: 118:72825
TITLE: Reversed phase planar chromatography of enantiomeric compounds with bovine serum albumin in the mobile phase
AUTHOR(S): Lepri, Luciano; Coas, Vanda; Desideri, Pier Giorgio; Pettini, Lilia
CORPORATE SOURCE: Dep. Public Health, Univ. Florence, Florence, 50121, Italy
SOURCE: J. Planar Chromatogr.--Mod. TLC (1992), 5(5), 364-7
CODEN: JPCTE5; ISSN: 0933-4173
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The chromatog. behavior of DL methylthiohydantoin and phenylthiohydantoin derivs. of amino acids, kynurenine, 3-(1-naphthyl)alanine, lactic acid derivs., alanine and leucine p-nitroanilides, and 2,2,2-trifluoro-1-(9-anthryl)ethanol has been extensively investigated on RP-18W/UV254 and Sil C18-50 UV254 plates developed with aq. org. mobile phases contg. bovine serum albumin (BSA) as a chiral agent. The success of enantiomeric sepn. is highly dependent on the type of the layer, the concn. of BSA, the org. modifier, and the pH of the mobile phase. High .alpha. and Rs values have been obtained for most sepns.
IT **1968-34-9**
RL: ANST (Analytical study); PROC (Process)
(resoln. of, by reversed-phase TLC using bovine serum albumin as mobile phase modifier)
RN 1968-34-9 CAPLUS
IT **28868-23-7 145552-40-5**
RL: ANST (Analytical study); PROC (Process)
(sepn. of, from enantiomer by reversed-phase TLC using bovine serum albumin as mobile phase modifier)
RN 28868-23-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

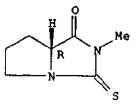
Absolute stereochemistry.

L12 ANSWER 34 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



RN 145552-40-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo-, (7aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



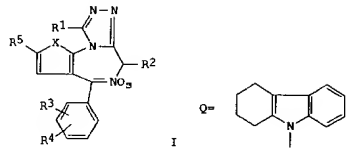
L12 ANSWER 35 OF 208 CAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1991:143456 CAPLUS
DOCUMENT NUMBER: 114:143456
TITLE: Preparation and formulation of (heterocyclylethynyl)-triazolo[4,3-a]benzodiazepines and -thieno[3,2-f][1,2,4] triazolo [4,3-a][1,4] diazepines and analogs as platelet activating factor antagonists
INVENTOR(S): Walser, Armin
PATENT ASSIGNEE(S): Hoffmann-La Roche, Inc., USA
SOURCE: U.S., 52 pp. Cont.-in-part of U.S. Ser. No. 227,948, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4959361	A	19900925	US 1988-252964	19881003
ZA 8809116	A	19890830	ZA 1988-9116	19881205
CA 1327570	A1	19940308	CA 1988-585981	19881215
DK 8807040	A	19890619	DK 1988-7040	19881216
FI 8805820	A	19890619	FI 1988-5820	19881216
FI 88799	B	19930331		
FI 88799	C	19930712		
NO 8805597	A	19890619	NO 1988-5597	19881216
NO 167920	B	19910916		
NO 167920	C	19911227		
AU 8826989	A1	19890629	AU 1988-26989	19881216
AU 612441	B2	19910711		
JP 01197484	A2	19890809	JP 1988-316555	19881216
JP 07025762	B4	19950322		
HU 50823	A2	19900328	HU 1988-6449	19881216
HU 204273	B	19911230		
ES 2056889	T3	19941016	ES 1988-121165	19881216
RU 2071962	C1	19970120	RU 1988-4613119	19881216
CN 1034722	A	19890816	CN 1988-108697	19881217
CN 1031057	B	19960221		
RU 2094436	C1	19971027	RU 1992-5010684	19920131

PRIORITY APPLN. INFO.: US 1987-134726 19871218
US 1988-227948 19880803
OTHER SOURCE(S): MARPAT 114:143456
GI

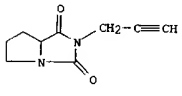
L12 ANSWER 35 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



I

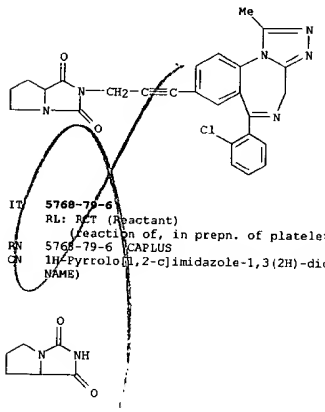
AB The title compds. [I; R1 = alkyl, alkoxy, CF3; R2 = H, alkyl, alkoxy, OH, AcO; R3, R4 = H, Cl, F, alkyl, alkoxy; R5 = R6(CH2)nC.tplbond.C, R7O(CH2)mC.tplbond.C; R6, R7 = aryl, heterocyclyl; X = CH:CH, S; m = 1, 2; n = 0-2; s = 0, 1] were prepd. Thus, I (R1 = Me, R2 = R3 = H, R4 = 2-Cl, R5 = iodo, X = S, s = 0) was stirred 20 h with RCH2C.tplbond.CH (R = tetrahydrocarbazolo group Q) in DMF contg. Et3N, CuI, Ph3P, and Pd(OAc)2 to give I (R5 = C.tplbond.CCH2Q; R1, R2, R3, R4, X, s = same as above) which had ID50 of 0.006 mg/kg orally against platelet activating factor-induced bronchoconstriction in guinea pigs.

IT **125030-31-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and reaction of, in prepn. of platelet activating factor antagonist)
RN 125030-31-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-(2-propynyl)-(9CI) (CA INDEX NAME)



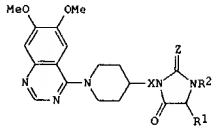
IT **132456-32-7P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as platelet activating factor antagonist)
RN 132456-32-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[3-[6-(2-chlorophenyl)-1-methyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepin-8-yl]-2-

L12 ANSWER 35 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
propynyl]tetrahydro- (9CI) (CA INDEX NAME)



IT **5768-79-6**
RL: RCT (Reactant)
(reaction of, in prepn. of platelet activating factor antagonists)
RN 5768-79-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro- (9CI) (CA INDEX NAME)

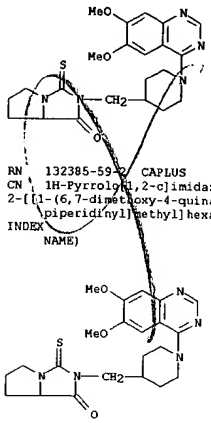
L12 ANSWER 36 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1991:122268 CAPLUS
DOCUMENT NUMBER: 114:122268
TITLE: Studies on cardiotonic agents. IV. Synthesis of novel 1-(6,7-dimethoxy-4-quinazolinyl)piperidine derivatives carrying substituted hydantoin and 2-thiohydantoin rings
AUTHOR(S): Nomoto, Yuji; Takai, Haruki; Hirata, Tadashi; Teranishi, Masayuki; Ohno, Tetsuji; Kubo, Kazuhiro
CORPORATE SOURCE: Tokyo Res. Lab., Kyowa Hakko Kogyo Co., Ltd., Machida, 194, Japan
SOURCE: Chem. Pharm. Bull. (1990), 38(11), 3014-19
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:122268
GI



I

AB A series of 6,7-dimethoxy-4-[4-[(5-oxo-2-thioxoimidazol-1-yl)alkyl]piperidin-1-yl]quinazoline derivs. or 6,7-dimethoxy-4-[4-[(2,5-dioxoimidazol-1-yl)alkyl]piperidin-1-yl]quinazoline derivs. I (R1 = H, Me, Pr, CH2CH2SMe, Me2CH, CH2Ph, etc.; R2 = H, Me; X = CH2, CH2CH2, CH2CH2CH2; Z = O, S) were prepd. Thus, 6,7-dimethoxy-4-[4-(aminoalkyl)piperidin-1-yl]quinazolines were condensed with protected amino acids and the resp. products were deprotected and treated with N,N'-carbonylimidazole to give I (same R1, R2, X; Z = O) or condensed with CS2 to give I (same R1, R2, X; Z = S). I had pos. cardiotonic activity in dogs.
IT **132385-58-1P 132385-59-2P 132486-81-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L12 ANSWER 36 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
RN 132385-58-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-[[1-(6,7-dimethoxy-4-quinazolinyl)-4-piperidinyl]methyl]hexahydro-3-thioxo- (9CI) (CA INDEX NAME)



RN 132385-59-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-[[1-(6,7-dimethoxy-4-quinazolinyl)-4-piperidinyl]methyl]hexahydro-3-thioxo-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 132486-81-8 CAPLUS

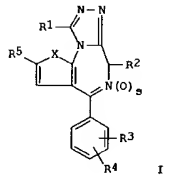
L12 ANSWER 37 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1990:118862 CAPLUS
DOCUMENT NUMBER: 112:118862
TITLE: Preparation and formulation of triazolodiazepine derivatives as platelet activator factor antagonists
INVENTOR(S): Walser, Armin
PATENT ASSIGNEE(S): Hoffmann-La Roche, F., und Co. A.-G., Switz.
SOURCE: Eur. Pat. Appl., 70 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 320992	A2	19890621	EP 1988-121165	19881216
EP 320992	A3	19910109		
EP 320992	B1	19940727		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
ZA 8809116	A	19890830	ZA 1988-9116	19881205
CA 1327570	A1	19940308	CA 1988-585981	19881215
DK 8807040	A	19890619	DK 1988-7040	19881216
FI 8805820	A	19890619	FI 1988-5820	19881216
FI 88799	B	19930331		
FI 88799	C	19930712		
NO 8805597	A	19890619	NO 1988-5597	19881216
NO 167920	B	19910916		
NO 167920	C	19911227		
AU 8826989	A1	19890629	AU 1988-26989	19881216
AU 612441	B2	19910711		
JP 01197484	A2	19890809	JP 1988-316555	19881216
JP 07025762	B4	19950322		
HU 50823	A2	19900328	HU 1988-6449	19881216
HU 204273	B	19911230		
ES 2056889	T3	19941016	ES 1988-121165	19881216
RU 2071962	C1	19970120	RU 1988-4613119	19881216
CN 1034722	A	19890816	CN 1988-108697	19881217
CN 1031057	B	19960221		
RU 2094436	C1	19971027	RU 1992-5010684	19920131

PRIORITY APPLN. INFO.: US 1987-134726 19871218
US 1988-227948 19880803

GI

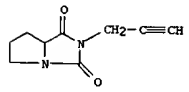
L12 ANSWER 37 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



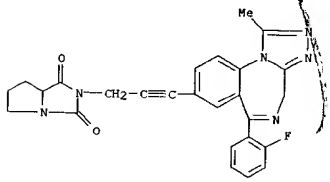
I

AB Title compds. [I; R1 = alkyl, alkoxy, F3C; R2 = H, alkyl, alkoxy, HO, alkanoyloxy; R3,R4 = H, Cl, F, alkyl, alkoxy; R5 = R6(CH2)nC.tplbond.C, R6,R7 = aryl, heterocyclyl; X = CH:CH, S; m = 1,2; n = 0-2; s = 0,1, with the proviso that when s = 1, R2 .noteq. HO, alkoxy, alkanoyloxy; when n = 0, R6 must be attached through a C to C bond, and that R7 is always attached through a C to O bond] their enantiomers, racemates and pharmaceutically acceptable acid addn. salts thereof, are prepd. I are useful in diseases characterized by excess platelet activating factor (PAF) or for prevention and treatment of cardiovascular disease, pulmonary disease, immunolog. disorder, inflammatory disease, dermatol. disorders and transplant rejection. 4-(2-Chlorophenyl)-2-iodo-9-methyl-6H-thieno[3,2-f][1,2,4]triazolo[4,3-a]diazepine was reacted with 1-(2-propynyl)-1H-indazole to give I (R1 = Me; R2, R4 = H; R3 = 2-Cl; R5 = [3-(1H-indazol-1-yl)-1-propynyl]; X = S; s = 0 (II). II inhibited PAF binding to dog platelets with an IC50 of 1.0 mM and inhibited of PAF-induced bronchoconstriction in guinea pigs with an i.v. ID50 of 0.002 mg/kg. An oral suspension comprised 2-[3-[4-(2-chlorophenyl)-9-methyl-6H-thieno[3,2-f][1,2,4]triazolo[4,3-a]diazepin-2-yl]-2-propynyl]-1H-benz[de]isoquinoline-1,3(2H)-dione 5.0, hydroxypropylmethyl cellulose 8.0, polysorbate 80 0.5 g and distd. water to 100 mL.
IT **125030-31-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, in prepn. of triazolodiazepine platelet activating factor antagonists)
RN 125030-31-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-(2-propynyl)-(9CI)
(CA INDEX NAME)

L12 ANSWER 37 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

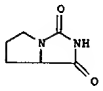


IT **125055-08-5P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as platelet activating factor antagonist)
RN 125055-08-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[3-[6-(2-fluorophenyl)-1-methyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepin-8-yl]-2-propynyl]tetrahydro- (9CI) (CA INDEX NAME)

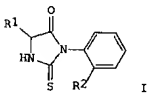


IT **5768-79-6**
RL: RCT (Reactant)
(propargylation of)
RN 5768-79-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro- (9CI) (CA INDEX NAME)

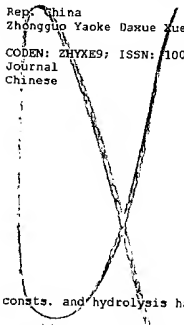
L12 ANSWER 37 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



L12 ANSWER 38 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1990:48249 CAPLUS
DOCUMENT NUMBER: 112:48249
TITLE: Determination of hydrolysis rate and preliminary structure-activity relationship of thiohydantoin derivatives
AUTHOR(S): Xu, Guoyou; Yu, Zhengwei; Peng, Sixun
CORPORATE SOURCE: Dep. Med. Chem., China Pharm. Univ., Nanjing, Peop. Rep. China
SOURCE: Zhongguo Yaoke Daxue Xuebao (1989), 20(4), 199-202
CODEN: ZHYXE9; ISSN: 1000-5048
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
GI



I

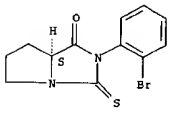


AB The hydrolysis rate consts. and hydrolysis half-lives of 22 thiohydantoin derivs. (I; R1 = amino acids; R2 = H, OMe, Cl or Br) were detd. in MeCN (12%)-phosphate buffer (0.02M), pH 7.4, at 10.degree., with a UV spectrophotometer to investigate the relationship between the hydrolysis rate consts. and the antinociceptive activity of these compds. Preliminary studies on the structure-activity relationship showed that the thiohydantoin derivs. with potent antinociceptive activity might be more water-sol., rapidly ring-opened and hydrolyzed, and the most active had a structure related to that of enkephalinase.

IT **124916-33-2 124917-76-6 124917-77-7**
RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(analgesic activity of, hydrolysis rate and structure in relation to)
RN 124916-33-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(2-bromophenyl)hexahydro-3-thioxo-, (S)- (9CI) (CA INDEX NAME)

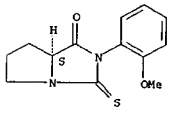
Absolute stereochemistry.

L12 ANSWER 38 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



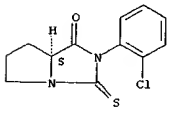
RN 124917-76-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-(2-methoxyphenyl)-3-thioxo-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

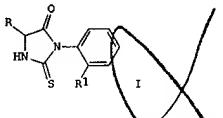


RN 124917-77-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(2-chlorophenyl)hexahydro-3-thioxo-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

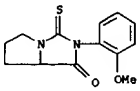


L12 ANSWER 39 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1989:633511 CAPLUS
DOCUMENT NUMBER: 111:233511
TITLE: Synthesis and antinociceptive activity of thiohydantoin derivatives
AUTHOR(S): Xu, Guoyou; Yu, Zhengwei; Peng, Sixun
CORPORATE SOURCE: Dep. Med. Chem., China Pharm. Univ., Nanjing, Peop. Rep. China
SOURCE: Zhongguo Yaoke Daxue Xuebao (1988), 19(4), 245-8
CODEN: ZHYXE9; ISSN: 1000-5048
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
GI

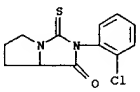


AB A series of thiohydantoin amino acid derivs. I (R = amino acid side chain ; R = OMe, Cl, Br) were designed according to the inhibitory mechanism of enkephalinase, and then synthesized with certain DL-amino acids and corresponding o-substituted Ph isothiocyanates to search for new potent analgesics. Studies on the antinociceptive activity were extended to these 19 newly synthesized thiohydantoin derivs. The mouse hot plate test (in vivo) showed that the antinociceptive activity of I (R = histidine side chain ; R = o-OMe) (100 mg/kg, i.p.) might be compared with that of morphine hydrochloride (20 mg/kg, i.p.).
IT **123861-09-6P 123861-15-4P 123861-21-2P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and analgesic activity of)
RN 123861-09-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-(2-methoxyphenyl)-3-thioxo-
(9CI) (CA INDEX NAME)

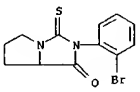
L12 ANSWER 39 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



RN 123861-15-4 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(2-chlorophenyl)hexahydro-3-thioxo-
(9CI) (CA INDEX NAME)



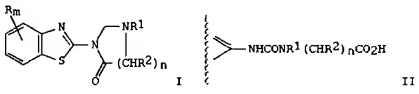
RN 123861-21-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(2-bromophenyl)hexahydro-3-thioxo-
(9CI) (CA INDEX NAME)



L12 ANSWER 40 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1983:198237 CAPLUS
DOCUMENT NUMBER: 98:198237
TITLE: Benzothiazole derivatives
PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

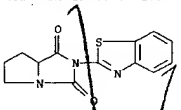
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 57175189	A2	19821028	JP 1981-60368	19810421
JP 63032073	B4	19880628		

GI

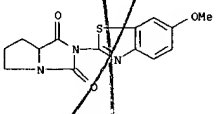


AB Thirty benzothiazole derivs. I [R = alkyl, alkoxy, halo, NO2; R1 = H, alkyl, alkanoyl, alkoxycarbonyl; R2 = H, alkyl, MeSCH2CH2, aralkyl; R1R2 = (CH2)p (p = 3, 4)); m = 0-4; n = 1, 2] were prepd. by cyclization of II.
I had platelet aggregation inhibitory, hypotensive, herbicidal, and antibacterial activities (no data). Thus, stirring II (Rm = 6-EtO, R1 = Me, R2 = H, m = n = 1) in Ac2O 2 h at 70.degree. gave 90.7% I (Rm = 6-EtO, R1 = Me, R2 = H, m = n = 1).
IT **85102-12-1P 85102-14-3P 85102-15-4P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and biol. activities of)
RN 85102-12-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(2-benzothiazolyl)tetrahydro-
(9CI) (CA INDEX NAME)

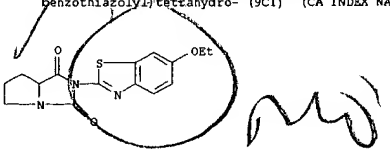
L12 ANSWER 40 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



RN 85102-11-3 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-(6-methoxy-2-benzothiazolyl)- (9CI) (CA INDEX NAME)



RN 85102-15-4 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(6-ethoxy-2-benzothiazolyl)tetrahydro- (9CI) (CA INDEX NAME)



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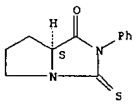
L12 ANSWER 41 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 2000:202584 CAPLUS
DOCUMENT NUMBER: 132:334401
TITLE: Solid phase synthesis of hydantoins by thermal cyclization and screening of reaction conditions using APOS 1200
AUTHOR(S): Karnbrock, Wilhelm; Deeg, Martin; Gerhardt, Jurgen; Rapp, Wolfgang
CORPORATE SOURCE: Rapp Polymere GmbH, Tubingen, D-72072, Germany
SOURCE: Mol. Diversity (2000), Volume Date 1998, 4(3), 165-171
CODEN: MODIF4; ISSN: 1381-1991
PUBLISHER: Kluwer Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A novel strategy for solid-phase synthesis of hydantoins with high optical purity is described using a thermal pH-neutral cyclization and simultaneous release from resin. Even hydantoins bearing a pH-sensitive side chain (protection) are available. The reaction conditions are well screened applying the parallel org. synthesizer APOS 1200.
IT **29635-99-2P 70741-88-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(solid phase synthesis of hydantoins by thermal cyclization)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

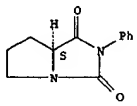
Absolute stereochemistry.



RN 70741-88-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-phenyl-, (7aS)-(9CI) (CA INDEX NAME)

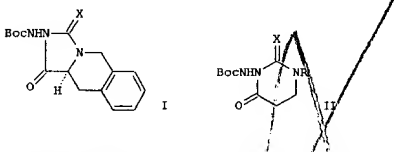
Absolute stereochemistry.

L12 ANSWER 41 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



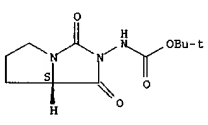
REFERENCE COUNT: 14
REFERENCE(S):
(4) Dressman, B; Tetrahedron Lett 1996, V37, P937 CAPLUS
(6) Gong, Y; J Org Chem 1998, V63, P3081 CAPLUS
(7) Gremlich, H; Appl Spectrosc 1996, V50, P532 CAPLUS
(8) Hanessian, S; Tetrahedron Lett 1996, V37, P5835 CAPLUS
(10) Joshi, P; J Heterocyc Chem 1979, V16, P607 CAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 42 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 2000:158959 CAPLUS
DOCUMENT NUMBER: 132:293732
TITLE: An efficient one-pot synthesis of 3-aminohydantoin and 3-aminodihydrouracil derivatives
AUTHOR(S): Wu, Shengde; Janusz, John M.; Sheffer, James B.
CORPORATE SOURCE: Procter and Gamble Pharmaceuticals, Health Care Research Center, Mason, OH, 45040, USA
SOURCE: Tetrahedron Lett. (2000), 41(8), 1159-1163
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:293732
GI



AB Title compds. such as I (X = O, S) and II (X = O, S; R = benzyl, 2-furylmethyl, Bu, Ph) were prepd. from 1,1'-carbonyldiimidazole or 1,1'-thiocarbonyldiimidazole, tert-Bu carbazate, and amino acid esters.
IT **264195-27-9P 264195-28-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of 3-aminohydantoin and 3-aminodihydrouracil derivs.)
RN 264195-27-9 CAPLUS
CN Carbamic acid, [(7aS)-tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

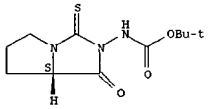
Absolute stereochemistry.



RN 264195-28-0 CAPLUS
CN Carbamic acid, [(7aS)-tetrahydro-1-oxo-3-thioxo-1H-pyrrolo[1,2-c]imidazol-

L12 ANSWER 42 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
2(3H)-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 20
REFERENCE(S):
(1) Bernard, L; FR 2000801 1969 CAPLUS
(2) Davidson, J; J Chem Soc 1964, P4646 CAPLUS
(3) Gante, J; Chem Ber 1964, V97, P994 CAPLUS
(4) Gillis, B; J Heterocycl Chem 1971, V8, P339 CAPLUS
(5) Kiec-Kononowicz, K; Pol J Chem 1984, V58, P585 CAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 43 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 2000:43953 CAPLUS
DOCUMENT NUMBER: 132:251408
TITLE: Development of an Amino Acid Sequence and D/L-Configuration Determination Method of Peptide with a New Fluorescence Edman Reagent, 7-Methylthio-4-(2,1,3-benzoxadiazolyl) Isothiocyanate
AUTHOR(S): Toriba, Akira; Adzuma, Kentaro; Santa, Tomofumi; Imai, Kazuhiro
CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences, The University of Tokyo, Tokyo, 113-0033, Japan
SOURCE: Anal. Chem. (2000), 72(4), 732-739
CODEN: ANCHAM; ISSN: 0003-2700
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB On the basis of the relationship between the fluorescence characteristics of the benzofurazan compds. and the Hammett consts. (.sigma.p), a new fluorescence Edman reagent, 7-methylthio-4-(2,1,3-benzoxadiazolyl) isothiocyanate (MTBD-NCS) was designed and synthesized. MTBD-thiohydantoin (TH)-amino acid derivs. produced by the Edman sequencing method gave fluorescence, whereas other degrdn. byproducts such as MTBD-thiocarbamoyl (TC)- or carbamoyl (CA)-amino acids did not fluoresce. MTBD-NCS was applicable as an Edman sequencing reagent to the simultaneous detn. of both the sequence and D/L-configuration of amino acids in peptides. Boron trifluoride (BF3) and HCl/methanol were adopted as the cyclization/cleavage and conversion reagents to suppress the amino acid residue racemization. The MTBD-TH-amino acids were sepd. on a reversed-phase column for amino acid sequencing, and their enantiomers were resolved on two types of polysaccharide-based chiral stationary phases for D/L-configuration detn. The method was successfully applied to the sequence and D/L-configuration detn. of D-amino acid-contg. peptide [D-Ala2]-deltorphin II.

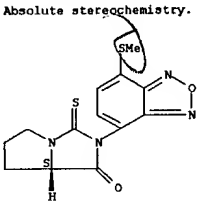
IT **262369-46-0P 262369-47-1P**
RL: ANT (Analyte); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)
(amino acid sequence and configuration detn. method of peptide with methylthio(benzoxadiazolyl) isothiocyanate)

RN 262369-46-0 CAPLUS

L12 ANSWER 43 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

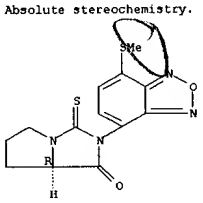
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-[7-(methylthio)-2,1,3-benzoxadiazol-4-yl]-3-thioxo-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 262369-47-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-[7-(methylthio)-2,1,3-benzoxadiazol-4-yl]-3-thioxo-, (7aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 26
REFERENCE(S):
(1) Cavins, J; Anal Biochem 1970, V35, P489 CAPLUS
(2) Edman, P; Acta Chem Scand 1950, V4, P283 CAPLUS
(3) Erspamer, V; Proc Natl Acad Sci USA 1989, V86, P5188 CAPLUS
(4) Fujii, N; Biochim Biophys Acta 1994, V1204, P157 CAPLUS
(5) Fujii, N; J Biochem 1994, V116, P663 CAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

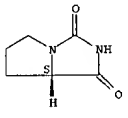
L12 ANSWER 44 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1998:593229 CAPLUS
DOCUMENT NUMBER: 129:277644
TITLE: Recognition over footprint cavities
AUTHOR(S): Morihara, Kensaku
CORPORATE SOURCE: Department of Chemistry, Faculty of Science, Nara Women's University, Nara, 630, Japan
SOURCE: ACS Symp. Ser. (1998), 703(Molecular and Ionic Recognition with Imprinted Polymers), 300-313
CODEN: ACSMC8; ISSN: 0097-6156
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB "Footprint cavities" are mol.-imprinted sites on an aluminum ion doped silica gel surface with complementary cavities which also possess Lewis acid sites. Like catalytic antibodies, these sites exhibit catalytic behavior with tailorable selectivity. This distinguishes the footprint cavities from the imprinted adsorption sites in vinyl polymers. These sites catalyze substrate-specific and stereo-selective acyl transfer reactions, condensations, racemizations, and redns. Our studies of these reactions reveal that the configuration of the template bound during imprinting predetermines the structure of the cavities and the orientation of substrate mols. bound within the cavities det. the mechanisms of the catalyzed reactions. Thus, our investigation of these phenomena provides useful information for the design of templates to allow construction of cavities capable of fine mol. recognition and specific catalysis.

IT **40856-87-9P 214066-57-6P**
RL: PUR (Purification or recovery); PREP (Preparation)
(mol. recognition over footprint cavities for catalyst)

RN 40856-87-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-, (7aS)- (9CI) (CA INDEX NAME)

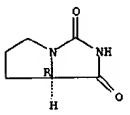
Absolute stereochemistry.



RN 214066-57-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-, (7aR)- (9CI) (CA

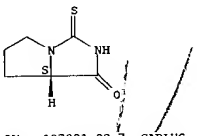
L12 ANSWER 44 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
INDEX NAME)

Absolute stereochemistry.



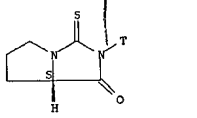
L12 ANSWER 45 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

Absolute stereochemistry.



RN 197021-29-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-t-3-thioxo-, (S)- (9CI)
(CA
INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 45 OF 208 CAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1997:650335 CAPLUS
DOCUMENT NUMBER: 127:293646
TITLE: Method for preparing amino acid thiohydantoins
INVENTOR(S): Inglis, Adam; Tseng, Albert Peng Sheng; Antonova, Olga V.
PATENT ASSIGNEE(S): Garvan Institute of Medical Research, Australia; Inglis, Adam; Tseng, Albert Peng Sheng; Antonova, Olga V.
SOURCE: PCT Int. Appl., 25 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9735844	A1	19971002	WO 1997-AU200	19970327
W: AU, CA, JP, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9721440	A1	19971017	AU 1997-21440	19970327
PRIORITY APPLN. INFO.:			AU 1996-8963	19960327
			WO 1997-AU200	19970327

AB Method of prepg. unlabeled or radiolabeled amino acid thiohydantoins, either in isolation or as the C-terminal residue of a peptide comprising reacting the amino acid or the peptide in the presence of a strong acid with acetic anhydride, acetic acid or tritiated acetic acid and a thiocyanate or an isothiocyanate, the reaction carried out either in liq. or vapor phase. Thus, an N-acetylamino acid or peptide was treated with ammonium thiocyanate, acetic anhydride, and tritiated acetic acid (prepd. from acetic anhydride and tritiated water) in a screw-cap vial at room temp. overnight. The thiohydantoin was cleaved under anhyd. conditions using HCl in acetic acid (prepd. from acetyl chloride and tritiated water),.

IT **61160-12-1P 197021-29-7P**
RL: ANT (Analyte); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)
(method for prepg. amino acid thiohydantoins)

RN 61160-12-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-3-thioxo-, (7aS)- (9CI) (CA
INDEX NAME)

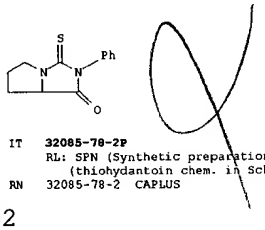
L12 ANSWER 46 OF 208 CAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1996:471996 CAPLUS
DOCUMENT NUMBER: 125:276449
TITLE: Studies in thiohydantoin chemistry. I. Some aspects of the Schlack-Kumpf reaction
AUTHOR(S): Duggan, Brendan M.; Laslett, Robert L.; Wilshire, John F. K.
CORPORATE SOURCE: Division of Biomolecular Engineering, CSIRO, Parkville, 3052, Australia
SOURCE: Aust. J. Chem. (1996), 49(5), 541-550
CODEN: AJCHAS; ISSN: 0004-9425
DOCUMENT TYPE: Journal
LANGUAGE: English

AB An investigation has been carried out into the Schlack-Kumpf reaction, i.e., the reaction of amino acids with a mixt. of acetic anhydride, acetic acid and sodium thiocyanate (occasionally ammonium thiocyanate was used). Particular emphasis was placed on the reactions with amino acids contg. sensitive or functional side chains, i.e., serine, threonine, arginine, proline, lysine, histidine, cysteine, and aspartic and glutamic acids. The reaction of serine, and of certain of its O- and N-substituted derivs., takes an unusual course to give an acetylated thiohydantoin deriv. of cysteine. Correspondingly, threonine gives an acetylated thiohydantoin deriv. of .beta.-methylcysteine. Similar reactions occurred with the 3-phenylthiohydantoin derivs. of serine and of threonine to give acetylated thiohydantoin derivs. of cysteine and of .beta.-methylcysteine, resp.

IT **4333-21-5**
RL: RCT (Reactant)
(thiohydantoin chem. in Schlack-Kumpf reaction of amino acids)

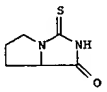
RN 4333-21-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo- (9CI) (CA
INDEX NAME)



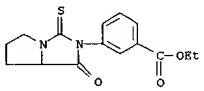
IT **32085-78-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(thiohydantoin chem. in Schlack-Kumpf reaction of amino acids)

RN 32085-78-2 CAPLUS

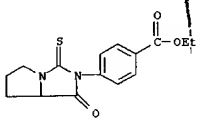
L12 ANSWER 46 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-3-thioxo- (9CI) (CA INDEX NAME)



L12 ANSWER 47 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

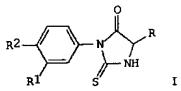


L12 ANSWER 47 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1996:109742 CAPLUS
DOCUMENT NUMBER: 124:250548
TITLE: Synthesis of thiohydantoin derivatives as analgesics
AUTHOR(S): Li, Zhiyu; Yu, Zhengwei; Peng, Sixun
CORPORATE SOURCE: Dep. Pharmaceutical Chem., China Pharmaceutical Univ., Nanjing, 210009, Peop. Rep. China
SOURCE: Zhongguo Yaoke Daxue Xuebao (1995), 26(5), 257-8
CODEN: ZHYXE9; ISSN: 1000-5048
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB A series of thiohydantoin derivs. (.+-.) 5-amino acid residue-3-substituted-phenyl-2-thioxo-hydantoin (substituted-PTH-AA) were designed based on the inhibitory mechanism of enkephalinase and synthesized with DL-amino acids and corresponding substituted-Ph isothiocyanates. Studies on the antinociceptive activity were extended to those 25 novel synthesized thiohydantoin derivs. The mouse hot plate showed that in vivo the antinociceptive activity of P-EtOOC'-P TH-Ala (YL-2), m-EtOOC'-PTH-Phe(YL-12), m-EtOOC-PTH-Ala (YL-13), (50 mg kg-1, i.p.) was comparable with that of morphine hydrochloride (20 mg kg, i.p.).
IT **174910-21-5P 174910-23-7P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis of aminoacid thiohydantoin derivs. as analgesics)
RN 174910-21-5 CAPLUS
CN Benzoic acid, 4-(tetrahydro-1-oxo-3-thioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)-, ethyl ester (9CI) (CA INDEX NAME)



RN 174910-23-7 CAPLUS
CN Benzoic acid, 3-(tetrahydro-1-oxo-3-thioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)-, ethyl ester (9CI) (CA INDEX NAME)

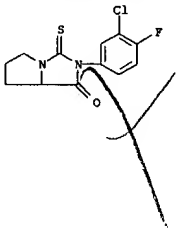
L12 ANSWER 48 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1992:524304 CAPLUS
DOCUMENT NUMBER: 117:124304
TITLE: Synthesis and antinociceptive activity of thiohydantoin derivatives
AUTHOR(S): Zhou, Jinpei; Yu, Zhengwei; Li, Minghua
CORPORATE SOURCE: Dep. Pharm. Chem., China Pharm. Univ., Nanjing, Peop. Rep. China
SOURCE: Zhongguo Yaoke Daxue Xuebao (1991), 22(6), 330-3
CODEN: ZHYXE9; ISSN: 1000-5048
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
GI



I

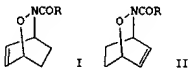
AB On the basis that the antinociceptive activity of some phenylthiohydantoin (PTH) compds. is due to the inhibition of enkephalinase, a series of amino acid derivs. (I; R = amino acid .alpha.-substituent, R1 = CF3 or Cl, R2 = H or F) was designed and synthesized in order to fine novel potent analgesics. Studies of antinociceptive activity were extended to these 17 newly synthesized thiohydantoin derivs. The mouse hot plate test showed that the antinociceptive activity of 3'-CF3-PTH-Ala (100 mg/kg, i.p.), 3'-Cl-4'-F-PTH-Ala (100 mg/kg, i.p.) and 3'-Cl-4'-F-PTH-Arg HCl (100 mg/kg, i.p.) was comparable with that of morphine hydrochloride (40 mg/kg, i.p.).
IT **143247-42-1P 143247-43-2P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. and analgesic activity of)
RN 143247-42-1 CAPLUS
RN 143247-43-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(3-chloro-4-fluorophenyl)hexahydro-3-thioxo- (9CI) (CA INDEX NAME)

L12 ANSWER 48 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



L12 ANSWER 49 OF 208 CAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1992:193444 CAPLUS
DOCUMENT NUMBER: 116:193444
TITLE: Asymmetric Diels-Alder cycloadditions with chiral carbamoyl dienophiles
AUTHOR(S): Defoin, Albert; Brouillard-Poichet, Agnes; Streith, Jacques
CORPORATE SOURCE: Ec. Natl. Super. Chim., Univ. Haute-Alsace, Mulhouse, F-68093, Fr.
SOURCE: Helv. Chim. Acta (1992), 75(1), 109-23
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:193444
GI



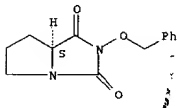
I II

AB Chiral acyl nitroso dienophiles RCON:O [R = (-)-(S)-(hydroxymethyl)-2-pyrrolidinyl, etc.], which were obtained from L-proline and D-mandelic acid, reacted with cyclohexa-1,3-diene to give the expected diastereoisomers I and II (same R). The d.e. values for these Diels-Alder reactions were moderate; they are related to the mol. stiffness of the dienophiles. The abs. configuration of the major cycloadducts was interpreted in terms of HOMO/LUMO interactions, the approach being endo and the acyl nitroso dienophiles reacting from their s-cis-conformation.

IT **140160-62-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrogenolysis of)
RN 140160-62-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-(phenylmethoxy)-, (S)- (9CI) (CA INDEX NAME)

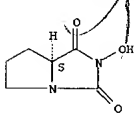
Absolute stereochemistry.

L12 ANSWER 49 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



IT **140160-63-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 140160-63-0 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-hydroxy-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



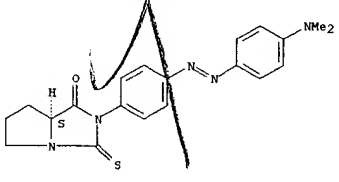
L12 ANSWER 50 OF 208 CAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1991:20542 CAPLUS
DOCUMENT NUMBER: 114:20542
TITLE: Capillary zone electrophoresis separation and laser-based detection of both fluorescein thiohydantoin and dimethylaminoazobenzene thiohydantoin derivatives of amino acids
AUTHOR(S): Waldron, Karen C.; Wu, Shaole; Earle, Colin W.; Harke, Heather R.; Dovichi, Norman J.
CORPORATE SOURCE: Dep. Chem., Univ. Alberta, Edmonton, AB, T6G 2G2, Can.
SOURCE: Electrophoresis (Weinheim, Fed. Repub. Ger.) (1990), 11(9), 777-80
CODEN: ELCTDN; ISSN: 0173-0835
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Capillary zone electrophoresis is employed for the sepn. and anal. of both fluorescein thiohydantoin and dimethylaminoazobenzene thiohydantoin derivs. of amino acids. Detection of minute amts. of these amino acid derivs. is an important milestone in the development of a high sensitivity protein sequencer. Current detection limits for the fluorescein deriv. is on the order of 10-21 mol whereas detection limits for the dimethylaminoazobenzene deriv. is on the order of 10-16 mol.

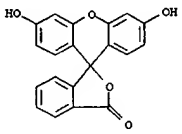
IT **103697-53-6 131069-17-5**
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, by capillary zone electrophoresis and laser-based fluorescence detection)
RN 103697-53-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-[4-[[4-(dimethylamino)phenyl]azo]phenyl]hexahydro-3-thioxo-, (S)- (9CI) (CA INDEX NAME)

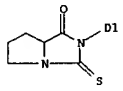
Absolute stereochemistry.
Double bond geometry unknown.



RN 131069-17-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-[3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5(or 6)-yl]hexahydro-3-thioxo-

L12 ANSWER 50 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
, (S)- (9CI) (CA INDEX NAME)

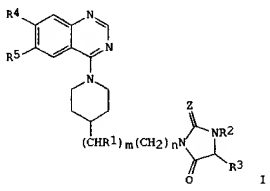




L12 ANSWER 51 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1988:522479 CAPLUS
DOCUMENT NUMBER: 109:122479
TITLE: Cardiotonics containing quinazoline derivatives
INVENTOR(S): Takai, Haruki; Nomoto, Yuji; Hirata, Tadashi; Ono, Tetsuji; Kubo, Kazuhiro
PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

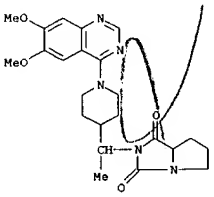
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63077874	A2	19880408	JP 1986-220048	19860918

OTHER SOURCE(S): MARPAT 109:122479
GI



AB Title compds. I [R1, R2 = H, alkyl; R3 = alkyl, (CH2)lQ [Q = OH, alkylthio, imidazolyl, (substituted) Ph, l = 1-5]; R2R3 = (CH2)3; R4, R5 = alkoxy; Z = O, S; m = 0, 1; n = 0-4] are prepd. and tested. A mixt. of 6,7-dimethoxy-4-[4-(aminomethyl)piperidino]quinazoline, Et3N, and CS2 in EtOH was stirred at room temp. for 2 h, followed by treatment with MeI for 1 h and with L-valine and Et3N at reflux for 10 h to give 41.1% I (R1 = R2 = H; R3 = Me2CH; R4 = R5 = MeO; Z = S; m = 1; n = 0) (II). II at 0.3 mg/kg i.v. showed 65.6 .+-. 3.4, 22.3 .+-. 7.0, and -28.7 .+-. 6.4% change in cardiomuscular contraction, heart beat, and blood pressure, resp. and

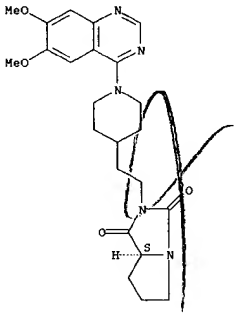
L12 ANSWER 51 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
its activity was sustained for >60 min in dogs, vs. 27.5 .+-. 11.7, 1.2 .+-. 1.2, and 2.2 .+-. 0.8%, resp. and 15 min for known 6,7-dimethoxy 4-[4-(3-butylureido)piperidino]quinazoline. Capsules (10,000) were formulated contg. II 100, Mg stearate 10, cryst. cellulose 640 and corn starch 250 g.
IT **105740-00-9P 106309-36-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as cardiotonic)
RN 105740-00-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[1-[1-(6,7-dimethoxy-4-quinazolinyl)-4-piperidinyl]ethyl]tetrahydro- (9CI) (CA INDEX NAME)



RN 106309-36-8 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[2-[1-(6,7-dimethoxy-4-quinazolinyl)-4-piperidinyl]ethyl]tetrahydro-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 51 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



L12 ANSWER 52 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1987:50243 CAPLUS
DOCUMENT NUMBER: 106:50243
TITLE: 4-Piperidinoquinazoline derivatives
INVENTOR(S): Takai, Haruki; Nomoto, Yuji; Hirata, Tadashi; Ono, Tetsuji; Kubo, Kazuhiro
PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61215389	A2	19860925	JP 1985-57474	19850320
US 4668683	A	19870526	US 1986-841656	19860320

PRIORITY APPLN. INFO.: JP 1985-57474 19850320
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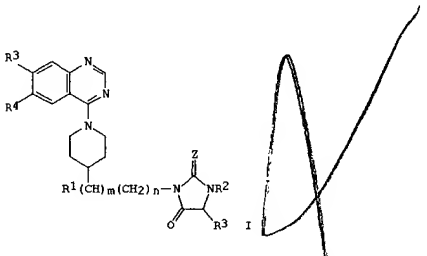
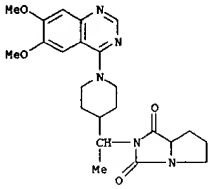


AB The title compds. [I; R1,R2 = H, alkyl; R3 = alkyl, (CH2)lR5 [l = 1-5, R5 = OH, alkylthio, 4-imidazolyl, (un)substituted phenyl] or R2R3 = (CH2)3; R3,R4 = alkoxy; Z = O, S; m = 0,1; n = 0-4], useful as cardiotonic agents, were prepd. Thus, a mixt. of 6,7-dimethoxy-4-[4-(aminomethyl)piperidino]quinazoline and CS2 in EtOH contg. Et3N was stirred at room temp. for 2 h. EtI was added to the mixt. and after 1 h at room temp. L-valine and Et3N were added. The resulting mixt. was refluxed for 10 h to give 41.1% (S)-I [R1(CH)m(CH2)n = CH2, R2 = H, R3 = CHMe2, R3 = R4 = OMe]. I at 0.3 mg i.v. increased the cardiomuscular contraction power by 67.8% (dp/dt max) in adult dogs.

IT **105740-00-9P 106309-36-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as cardiotonic agent)

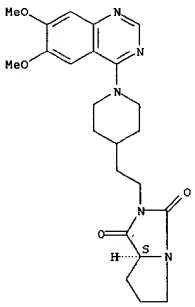
RN 105740-00-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[1-[1-(6,7-dimethoxy-4-quinazolinyl)-4-piperidinyl]ethyl]tetrahydro- (9CI) (CA INDEX NAME)



RN 106309-36-8 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[2-[1-(6,7-dimethoxy-4-quinazolinyl)-4-piperidinyl]ethyl]tetrahydro-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 52 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



L12 ANSWER 53 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1987:18603 CAPLUS
DOCUMENT NUMBER: 106:18603
TITLE: Antihypertensive and cardiotonic 4-(1-piperidinyl)quinazolines
INVENTOR(S): Takai, Haruki; Hirata, Tadashi; Ohno, Tetsuji; Kubo, Kazuhiro; Yuji, Nomoto
PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd. , Japan
SOURCE: Eur. Pat. Appl., 37 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 195667	A2	19860924	EP 1986-302033	19860319
EP 195667	A3	19861230		
EP 195667	B1	19890802		
R: DE, FR, GB, IT				

PRIORITY APPLN. INFO.: JP 1985-47474 19850320
GI

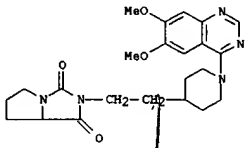
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

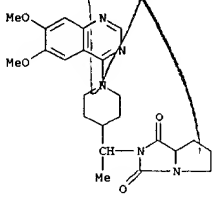
AB Title compds. [I; R1, R2 = H, alkyl; R3 = alkyl, (CH2)pR6; R2R3 = (CH2)3; R4 = alkoxy; R6 = OH, alkylthio, imidazolyl, (substituted) Ph; Z = O, S; m = 0, 1; n = 0-4; p = 1-5] are prepd. Thus, [(aminoethyl)piperidinyl]quinazoline II was treated with CS2 in the presence of Et3N-EtOH, followed by addn. of MeI and L-valine to give title compd. III. At 0.3 mg/kg i.v. in dogs, III gave a 28.7% decrease in blood pressure; the increase in cardiac contractile force lasted >60 min. I (R1 = R2 = H; R3 = CHMe2; R4 = R5 = OMe; m = 1; n = 0; Z = O) (IV) was formulated into tablets contg. IV 100, Mg stearate 4, cryst. cellulose 746 g/10,000 tablets.

IT **105739-99-9P 105740-00-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as antihypertensive and cardiotonic)

RN 105739-99-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[2-[1-(6,7-dimethoxy-4-quinazolinyl)-4-piperidinyl]ethyl]tetrahydro- (9CI) (CA INDEX NAME)

L12 ANSWER 53 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



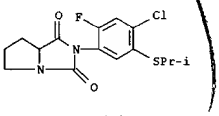


RN 105740-00-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[1-[1-(6,7-dimethoxy-4-quinazolinyl)-4-piperidinyl]ethyl]tetrahydro- (9CI) (CA INDEX NAME)

L12 ANSWER 54 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1987:18567 CAPLUS
DOCUMENT NUMBER: 106:18567
TITLE: N-Substituted (thio)urazoles and (thio)hydrantoins as herbicides
INVENTOR(S): Naohara, Tetsuo; Natsume, Fumitsugu; Ishii, Kazuo; Suzuki, Shigeru; Watanabe, Hisao; Ikeda, Osamu
PATENT ASSIGNEE(S): Mitsubishi Chemical Industries Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 19 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

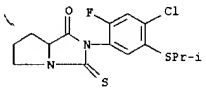
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61076487	A2	19860418	JP 1984-198206	19840921

GI For diagram(s), see printed CA Issue.
AB The title compds [I; R = H, cyano, alkenyl, alkynyl, (un)substituted alkyl; R1 = H, halo; Z, Z1 = O, S; X = halo, X1 = N, CH; n = 2-6] were prepd., typically by cyclocondensation of 1,2-polymethylenehydrazine derivs. II (R2 = alkyl) with anilines III. Thus, a mixt of II (R2 = Et, n = 4, Z = Z1 = O) and III (R = CHEtCONMe2, R1 = F, X = Cl) in pyridine was stirred for 24 h and the product refluxed with MeONa/MeOH to give I (R = CHEtCONMe2, R1 = F, Z = Z2 = O, X = Cl, X1 = N, n = 4). I were active against Rotala, etc., at 2.5-10 g/are.
IT **105447-29-8P 105470-45-9P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as herbicide)
RN 105447-29-8 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-[4-chloro-2-fluoro-5-[(1-methylethyl)thio]phenyl]tetrahydro- (9CI) (CA INDEX NAME)

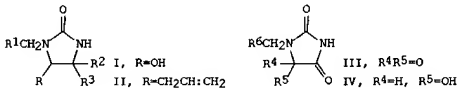


RN 105470-45-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-[4-chloro-2-fluoro-5-[(1-

L12 ANSWER 54 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
methylethyl)thio]phenyl]hexahydro-3-thioxo- (9CI) (CA INDEX NAME)

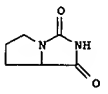


L12 ANSWER 55 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1985:6312 CAPLUS
DOCUMENT NUMBER: 102:6312
TITLE: Synthesis of substituted 2-imidazolidinones and annelated hydantoins via amidoalkylation transformations
AUTHOR(S): Liao, Zeng Kun; Kohn, Harold
CORPORATE SOURCE: Dep. Chem., Univ. Houston, Houston, TX, 77004, USA
SOURCE: J. Org. Chem. (1984), 49(25), 4745-52
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

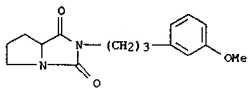


AB The synthetic utility of 4-hydroxy-2-imidazolidinone amidoalkylation reactions is limited by the propensity of the C-5 unsubstituted and C-5 monosubstituted adducts to undergo dehydration to yield 2-imidazolones. Two techniques are reported which avoided this competitive side reaction. The 1st approach utilized reactive allylsilanes. Treatment of substituted 4-hydroxy-2-imidazolidinones I (R1 = 3-MeOC6H4, PhCH2, R2 = R3 = Me; R1 = Ph, R2 = H, R3 = Me, H) with CH2:CHCH2SiMe3 under Lewis acid-mediated conditions led to high yields of the intermol. alkylation product II. The 2nd technique examd. the use of parabanic acid substrates as starting materials for the prepn. of annulated hydantoins. Treatment of III [R6 = PhCH2, 3,4-(MeO)2C6H3CH2, Ph(CH2)2, 3-MeOC6H4] with NaBH4 led to preferential redn. of the 5-carbonyl moiety to give IV. Cyclization of IV with (CF3CO)2O and F3CCO2H gave the fused-ring hydantoin, which was selectively reduced with LiAlH4 in the final step to yield the corresponding annulated 2-imidazolidinone.
IT **5768-79-6**
RL: RCT (Reactant)
(alkylation of, with phenylpropyl bromide deriv.)
RN 5768-79-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro- (9CI) (CA INDEX NAME)

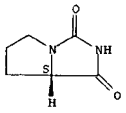
L12 ANSWER 55 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



IT **92763-94-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and lithium aluminum hydride redn. of)
RN 92763-94-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[3-(3-methoxyphenyl)propyl]- (9CI) (CA INDEX NAME)



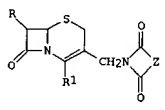
L12 ANSWER 56 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1981:443607 CAPLUS
DOCUMENT NUMBER: 95:43607
TITLE: Carbon-13 NMR spectra of hydantoins and 3-phenyl-2-thiohydantoins of amino acids
AUTHOR(S): Sobczyk, Katarzyna; Siemion, Ignacy Z.
CORPORATE SOURCE: Inst. Chem., Univ. Wroclaw, Wroclaw, 50383, Pol.
SOURCE: Pol. J. Chem. (1980), 54(9), 1833-40
CODEN: PJCHDQ
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Complete 13C NMR data for a series of hydantoins and 3-phenyl-2-thiohydantoins of amino acids are given. The hydantoins were prepd.
IT **31364-82-6 40856-87-9**
RL: PRP (Properties)
(carbon-13 NMR of)
RN 31364-82-6 CAPLUS
RN 40856-87-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-, (7aS)- (9CI) (CA INDEX NAME)
Absolute stereochemistry.



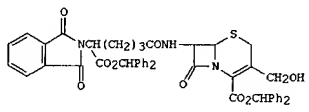
L12 ANSWER 57 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1980:426447 CAPLUS
DOCUMENT NUMBER: 93:26447
TITLE: Cephalosporin derivatives
INVENTOR(S): Horii, Satoshi; Fukase, Hiroshi; Mizokami, Nariaki
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 39 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 54092986	A2	19790723	JP 1977-160904	19771228

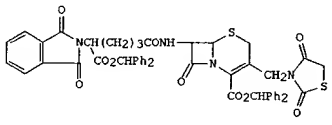
GI



I



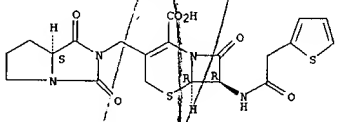
II



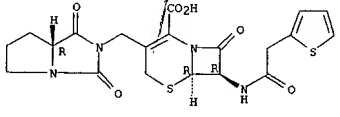
III

AB Thirty-six cephalosporin derivs. I [R = NH2, acylated NH2; R1 = CO2H, esterified CO2H; Z = CHR2S (R2 = H, alkyl), CH:NNR2, etc.] and their salts were prepd. Thus, stirring 1,3 g thiazolidine-2,4-dione with 8.5 g II, 2.9 g Ph3P, and 2 mL di-Et azodicarboxylate in THF 1.5 h gave 3.8 g III. Treating 2.4 g III with PCl5 and pyridine in CH2Cl2 at -20.degree. under N and 50 min at -12.degree., stirring with MeOH 30 min at -10.degree. and 1 h at room temp., and stirring with N HCl 45 min gave 1.18 g I (R = NH2, R1 = CO2CHPh2, Z = CH2S), which (405 mg) was stirred with F3CCO2H and PhOMe 20 min to give 279 mg I (R = NH2, R1 = CO2H, Z = CH2S) trifluoroacetate.

L12 ANSWER 57 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
IT **74046-88-1P 74046-89-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 74046-88-1 CAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 8-oxo-3-[(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)methyl]-7-[(2-thienylacetyl)amino]-, [6R-[3(S*),6.alpha.,7.beta.]]- (9CI) (CA INDEX NAME)
Absolute stereochemistry.



RN 74046-89-2 CAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 8-oxo-3-[(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)methyl]-7-[(2-thienylacetyl)amino]-, [6R-[3(R*),6.alpha.,7.beta.]]- (9CI) (CA INDEX NAME)
Absolute stereochemistry.

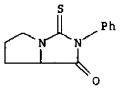


L12 ANSWER 58 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1980:193679 CAPLUS
DOCUMENT NUMBER: 92:193679
TITLE: Methylthiohydantoin amino acids: chromatographic separation and comparison to phenylthiohydantoin amino acids
AUTHOR(S): Horn, Marcus J.; Hargrave, Paul A.; Wang, Janet K.
CORPORATE SOURCE: Sequemat Inc., Watertown, MA, 02172, USA
SOURCE: J. Chromatogr. (1979), 180(1), 111-18
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Most phenylthiohydantoin (PTH) amino acids and most methylthiohydantoin (MTH) amino acids could be sepd. from 1 another by thin-layer chromatog. (TLC) using the same sequential development technique with the same 2 solvents. Similarly, a single solvent system could be used in high-performance liq. chromatog. (HPLC) to sep. most PTH-amino acids and most MTH-amino acids. When both TLC and HPLC sepns. were performed on a sample, all MTH- and PTH-amino acids could be uniquely identified. Since many solid-phase protein sequencing techniques generate both MTH- and PTH-amino acids, these anal. systems simplify identification of the amino acid derivs. Although the chromatog. properties of MTH- and PTH-amino acids were similar, they were not identical.

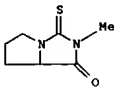
IT **4333-21-5 22712-58-9**
RL: ANT (Analyte); ANST (Analytical study)
(chromatog. of)

RN 4333-21-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo- (9CI) (CA INDEX NAME)



RN 22712-58-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo- (9CI) (CA

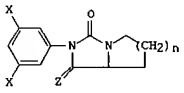
L12 ANSWER 58 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
INDEX NAME)



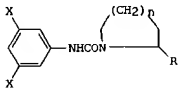
L12 ANSWER 59 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1978:443410 CAPLUS
DOCUMENT NUMBER: 89:43410
TITLE: 3-Phenylhydantoin derivatives
INVENTOR(S): Hisada, Yoshio; Takayama, Chiyozo; Kato, Yoshiro; Fujinami, Hikari
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
SOURCE: Japan. Kokai, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 53007697	A2	19780124	JP 1976-81372	19760707

GI



I, Z=O
IV, Z=NH



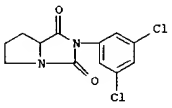
II, R=R1
IV, R=CN

AB Title derivs. I (X, n = Cl, 1; Cl, 2; Br, 1; Br, 2; resp.) were prepd. by intramol. cyclization of II (R1 = CO2H, alkoxycarbonyl) or III followed by hydrolysis of the resulting IV. Thus, 0.05 mol II (R = CO2H, X = Cl, n = 1) in 20% aq. HCl was refluxed 2 h to give 93% I (X = Cl, n = 1). Fungicidal data of I were given against Cochliobolus miyabeanus, Pellicularia sasakii, Sclerotinia sclerotiorum, etc.

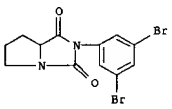
IT **60725-79-3P 66801-78-3P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and fungicidal activity of)

RN 60725-79-3 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(3,5-dichlorophenyl)tetrahydro- (9CI) (CA INDEX NAME)

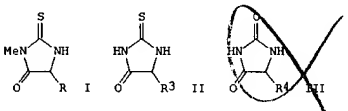
L12 ANSWER 59 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



RN 66801-78-3 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(3,5-dibromophenyl)tetrahydro- (9CI) (CA INDEX NAME)

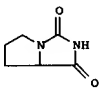


L12 ANSWER 60 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1977:568372 CAPLUS
DOCUMENT NUMBER: 87:168372
TITLE: Proton nuclear magnetic resonance studies on methylthiohydantoins, thiohydantoins, and hydantoins of amino acids
AUTHOR(S): Suzuki, Tateo; Tomioka, Tetsuhisa; Tuzimura, Katura
CORPORATE SOURCE: Fac. Agric., Tohoku Univ., Sendai, Japan
SOURCE: Can. J. Biochem. (1977), 55(5), 521-7
CODEN: CJBIAE
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

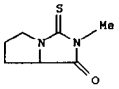


AB The proton NMR of methylthiohydantoins I [R = R1 [R1 = H, Me, CHMe2, CH2CHMe2, CHMeEt, CH2Ph, CH2C6H4OH-p, CH2CH2SMe, CH2CO2H, (CH2)3NHC(:NH)NH2, indol-3-ylmethyl, imidazol-4-ylmethyl], R2 [R2 = CH2CONH2, CH2CH2CONH2), CH2SH, CH2CH2CO2H, (CH2)4NHCSMe]], thiohydantoins II [R3 = R1, R2, CH2SCH2CO2H, (CH2)4NHAc], and hydantoins III [R4 = R1, CH2OH, CH(OH)Me, CH2SO3H, CH2CH2CO2H, (CH2)4NHAc] were given for the identification of the parent amino acid. The N- and C-terminal residues of Leu-Gly-Gly were detd. by an application of this proton NMR-hydantoin method.
IT **5768-79-6 22712-58-9**
RL: PRP (Properties)
(NMR of)
RN 5768-79-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro- (9CI) (CA INDEX NAME)

L12 ANSWER 60 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



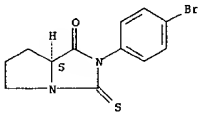
RN 22712-58-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo- (9CI) (CA INDEX NAME)



L12 ANSWER 61 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1977:1910 CAPLUS
DOCUMENT NUMBER: 86:1910
TITLE: Quantitative mass spectral identification of p-bromophenylthiohydantoins from Edman degradations by tetradeuterated internal standards
AUTHOR(S): Schneider, Michael; Tschesche, Harald
CORPORATE SOURCE: Inst. Org. Chem., Tech. Univ. Muenchen, Munich, Ger.
SOURCE: Hoppe-Seyler's Z. Physiol. Chem. (1976), 357(10), 1339-45
CODEN: HSZPAZ
DOCUMENT TYPE: Journal
LANGUAGE: English
AB P-bromophenylisothiocyanate is a reagent well suited for the Edman degrdn. of peptide chains, and the p-bromo substituent facilitates mass spectral identification of the p-bromophenylthiohydantoins obtained, due to its characteristic double peak. Quantitation of the amt. of p-bromophenylthiohydantoin obtained easily can be achieved in the parent mass spectrum by addn. of a known amt. of p-bromophenylthiohydantion-2H4 as an internal std. The tetradeuterated stds. give rise to mol. ion peaks 4 mass units higher than the corresponding undeuterated probe. Std. and probe volatilize almost equally well. The compn. in the vapor indicated by the H/D ratio reflects the M concns. over the entire range of probe evaporation. A procedure for the prepn. of the p-bromophenylisothiocyanate-2H4 and the resp. tetradeuterated amino acid p-bromophenylthiohydantoins is given.
IT **61357-79-7P 61357-94-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and mass spectroscopy of)
RN 61357-79-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(4-bromophenyl)hexahydro-3-thioxo-, (S)- (9CI) (CA INDEX NAME)

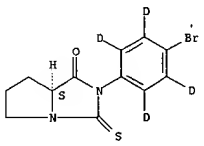
Absolute stereochemistry.

L12 ANSWER 61 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



RN 61357-94-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(4-bromophenyl-2,3,5,6-d4)hexahydro-3-thioxo-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 62 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1975:118174 CAPLUS
DOCUMENT NUMBER: 82:118174
TITLE: Photographic silver halide emulsion and light-sensitive material prepared from it
INVENTOR(S): Okumura, Akio; Sato, Akira; Ichijima, Seiji; Shiba, Keisuke; Nakazyo, Kiyoshi
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd.
SOURCE: Ger. Offen., 55 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2423820	A1	19741205	DE 1974-2423820	19740516
JP 50006341	A2	19750123	JP 1973-54456	19730516
US 4012259	A	19770315	US 1974-469923	19740514
GB 1439095	A	19760609	GB 1974-21921	19740516

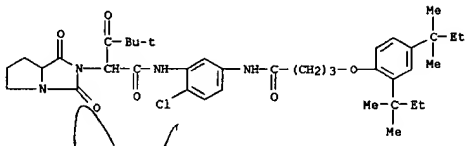
PRIORITY APPLN. INFO.: JP 1973-54456 19730516

AB The ketomethylene color formers contg. in their coupling position a 2,5-dioxo-1-imidazolidinyl group are described. Thus, .alpha.-pivaloyl-.alpha.-(2,5-dioxo-3,4-trimethylene-1-imidazolinyl)-2'-chloro-5'-[.gamma.-(2,4-di-tert-amylphenoxy)-butyramido]acetanilide was synthesized from the parent compd. by exchanging a Cl atom by 2,5-dioxo-3,4-trimethyleneimidazolidine. Comparison of a processed film contg. this coupler in a Ag(Br,I) emulsion with an analog in which the imidazolinyl residue carried a 3-Me group, instead of the 3,4-trimethylene group, revealed favorable sensitometric results and more complete removal of image Ag in a bleach soln.

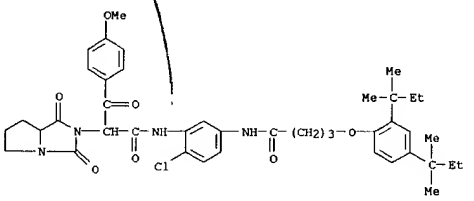
IT **54709-31-8 54709-32-9**
RL: TEM (Technical or engineered material use); USES (Uses)
(photog. yellow coupler)

RN 54709-31-8 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-2(3H)-acetamide, N-[5-[[4-[2,4-bis(1,1-dimethylpropyl)phenoxy]-1-oxobutyl]amino]-2-chlorophenyl]-.alpha.-(2,2-dimethyl-1-oxopropyl)tetrahydro-1,3-dioxo- (9CI) (CA INDEX NAME)

L12 ANSWER 62 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



RN 54709-32-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-2(3H)-acetamide, N-[5-[[4-[2,4-bis(1,1-dimethylpropyl)phenoxy]-1-oxobutyl]amino]-2-chlorophenyl]tetrahydro-.alpha.-(4-methoxybenzoyl)-1,3-dioxo- (9CI) (CA INDEX NAME)

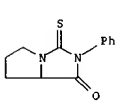


L12 ANSWER 63 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1972:72760 CAPLUS
DOCUMENT NUMBER: 76:72760
TITLE: Metastable transistions in the mass spectra of methyl and phenylthiohydantoin derivatives of amino acids
AUTHOR(S): Sun, T.; Lovins, R. E.
CORPORATE SOURCE: Dep. Biochem., Univ. Georgia, Athens, Ga., USA
SOURCE: Org. Mass Spectrom. (1972), 6(1), 39-45
CODEN: ORMSBG
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The mass spectra of a number of methyl- (MTH) and phenylthiohydantoin (PTH) amino acid derivs. were obtained. The major metastable transitions occurring in the mass spectra of these derivs. were identified and measured. The major fragmentation pathways assocd. with the metastable transitions were outlined and discussed for each group of compds. Inspection of the metastable data has shown that there is at least one unique metastable transition occurring for each thiohydantoin deriv. which may be used to uniquely identify that deriv. in the presence of a mixt. of thiohydantoin derivs. obtained from the Edman degradation of a peptide or protein. The use of metastable ions to uniquely identify thiohydantoin derivs. in mixts. has proven useful in the identification of the MTH and PTH derivatives of glycine whose mol. ions are not unique and for resolving such ambiguities as occur for example in the mixt. of leucine and isoleucine.

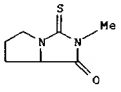
IT **4333-21-5 22712-58-9**
RL: PRP (Properties)
(mass spectrum of)

RN 4333-21-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo- (9CI) (CA INDEX NAME)



RN 22712-58-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo- (9CI) (CA

L12 ANSWER 63 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
INDEX NAME)

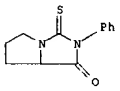


L12 ANSWER 64 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1972:32002 CAPLUS
DOCUMENT NUMBER: 76:32002
TITLE: Quantitative protein sequencing using mass spectrometry. Use of low ionizing voltages in mass spectral analysis of methyl- and phenylthiohydantoin amino acid derivatives
AUTHOR(S): Sun, T.; Lovins, R. E.
CORPORATE SOURCE: Dep. Biochem., Univ. Georgia, Athens, Ga., USA
SOURCE: Anal. Biochem. (1972), 45(1), 176-91
CODEN: ANBCA2
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The mass spectra of 18 methylthiohydantoin and 13 phenylthiohydantoin amino acid derivs. have been recorded at electron energies of 11, 20, and 70 eV. The spectra of the majority of the derivs. were decreased in complexity, in some cases contg. only the mol. ion. The mol. ion was generally the base peak of the low-voltage spectrum. The loss of sensitivity at lower ionizing voltages was measured for a no. of compds. and the sensitivity as measured by ion abundance was max. around 20 eV and decreased rapidly at lower energies. The use of low-energy electron impact ionization is compared to chem. ionization and the advantages and disadvantages discussed.

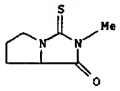
IT **4333-21-5 22712-58-9**
RL: PRP (Properties)
(spectrum of, low ionizing voltages in)

RN 4333-21-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo- (9CI) (CA INDEX NAME)



RN 22712-58-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo- (9CI) (CA INDEX NAME)

L12 ANSWER 64 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



L12 ANSWER 65 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 2001:489370 CAPLUS
DOCUMENT NUMBER: 135:76866
TITLE: Preparation of heterocyclic imino compounds as fungicides and insecticides for agricultural and horticultural use
INVENTOR(S): Niki, Toshio; Mizukoshi, Takashi; Takahashi, Hiroaki; Satow, Jun; Ogura, Tomoyuki; Yamagishi, Kazuhiro; Suzuki, Hiroyuki; Hayasaka, Fumio
PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 350 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

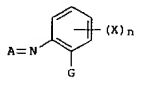
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001047888	A1	20010705	WO 2000-JP9411	20001228

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

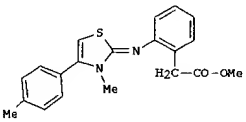
PRIORITY APPLN. INFO.: JP 1999-374040 A 19991228
JP 2000-239624 A 20000808
JP 2000-334442 A 20001101

GI

L12 ANSWER 65 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



I



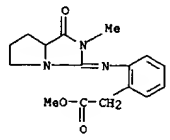
II

AB The title compds. I [G is a group of general formula BCOZ or the like; A is a 3- to 13-membered, mono-, di- or tricyclic ring which is composed of 3 to 13 atoms arbitrarily selected from among carbon, oxygen, sulfur and nitrogen, contains at least one heteroatom selected from among oxygen, sulfur and nitrogen, and may optionally have substituent(s), with the proviso that when A is a quinolone ring, the nitrogen atom of the ring is present at the .alpha.-position to the imino linkage; Z is OR1 or the like; B is CH2 or the like; n = 0 - 4; X is halogeno or the like; and R1 is hydrogen, C1-6 alkyl, C1-6haloalkyl, or the like] are prepd. The title compd. II at 500 ppm gave .gtoreq. 70% control of Pyricularia oryzae, Erysiphe graminis, Puccinia recondita, Leptosphaera nodorum, and Pseudoperonospora cubensis. II at 500 ppm gave .gtoreq. 70% control of leafhoppers.

IT **347876-23-7P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of heterocyclic imino compds. as fungicides and insecticides for agricultural and horticultural use)

RN 347876-23-7 CAPLUS
CN Benzeneacetic acid, 2-[(hexahydro-2-methyl-1-oxo-3H-pyrrolo[1,2-c]imidazol-3-ylidene)amino]-, methyl ester (9CI) (CA INDEX NAME)

L12 ANSWER 65 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



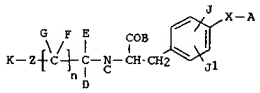
REFERENCE COUNT: 7
REFERENCE(S): (1) Geigy J R A-G; FR 1601535 A CAPLUS
(2) Geigy J R A-G; DE 1816700 C3 CAPLUS
(3) Geigy J R A-G; GB 1258920 A 1971 CAPLUS
(4) Maeda, R; Chem Pharm Bull 1983, V31(10), P3424
CAPLUS
(5) Nissan Chemical Industries Ltd; JP 06157478 A 1994
CAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 66 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 2001:380546 CAPLUS
DOCUMENT NUMBER: 134:367194
TITLE: Preparation of novel phenylalanine derivatives as .alpha.4-integrin inhibitors
INVENTOR(S): Tanaka, Yasuhiro; Yoshimura, Toshihiko; Izawa, Hiroyuki; Ejima, Chieko; Kojima, Mitsuhiko; Atake, Yuko; Nakanishi, Eiji; Suzuki, Nobuyasu; Makino, Shingo; Suzuki, Manabu; Murata, Masahiro
PATENT ASSIGNEE(S): Ajinomoto Co., Inc., Japan
SOURCE: PCT Int. Appl., 155 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001036376	A1	20010525	WO 2000-JP8152	20001120

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: JP 1999-328468 A 19991118
JP 2000-197139 A 20000629
OTHER SOURCE(S): MARPAT 134:367194
GI



I

L12 ANSWER 66 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

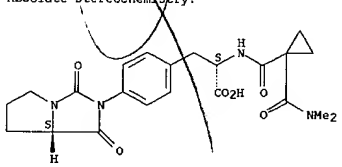
AB Phenylalanine derivs. represented by general formula (I) or pharmaceutically acceptable salts thereof [wherein X represents an interat. bond, O, OSO2, N-(un)substituted NH, NHCO, NHSO2, NHCONH, or NH(CS)NH, CO; Y and Z represent each CO, SO, or SO2; A represents a specific substituted Ph group or nitrogen-contg. heterocycle such as arom.-fused pyrimidinedione or pyrimidinone, 2,4- or 2,5-imidazolidinedione, or 5-imidazolone; C represents hydrogen, lower alkyl, lower alkenyl, lower alkynyl, cyclic alkyl-lower alkyl optionally contg. heteroatoms in the ring, aryl-lower alkyl, heteroaryl-lower alkyl; D and E represent each lower alkyl, lower alkenyl, lower alkynyl, cyclic alkyl-lower alkyl optionally contg. heteroatoms in the ring, aryl-lower alkyl, heteroaryl-lower alkyl, etc. or D and E may be bonded to each other to form a ring optionally contg. 1 or 2 O, N, or S in the ring; F and G represent each hydrogen, lower alkyl, lower alkenyl, lower alkynyl, cyclic alkyl-lower alkyl optionally contg. heteroatoms in the ring, aryl-lower alkyl, heteroaryl-lower alkyl, etc. or F and G may be bonded to each other to form a ring; n is from 0 to 2; K represents OR7, NR7R8, NHNR7R8, SR7, or R7; R7 and R8 represents H, lower alkyl, etc.; and J and J' represent each hydrogen, halogeno, lower alkyl, lower alkoxy, or NO2] are prepd. These derivs. and analogs thereof show an .alpha.4 integrin inhibitory activity and are usable as remedies for various diseases relating to .alpha.4 integrin, such as inflammatory diseases related to .alpha.4 integrin-dependent adhesion process, arthritis, inflammatory intestinal diseases, systemic lupus erythematosus, multiple sclerosis, Sjoegren syndrome, psoriasis, allergy, diabetes, cardiovascular diseases, arteriosclerosis, restenosis, tumor proliferation, tumor metastasis, or transplant rejection. Thus, O-(2,6-dichlorobenzyl)-L-tyrosine bound to Wang resin was allowed to react with diethylmalonic acid, HOAt, 2-dimethylaminoisopropyl chloride hydrochloride (DIC), and N-methyl-2-pyrrolidinone (NMP) at room temp. for 16 h, washed with DMF five times, and condensed with pyrroline using HOAt, DIC, and NMP, followed by oxidn. with OsO4 in dioxane at room temp. for 16 and resin-cleavage in aq. CF3CO2H to give N-[2-[(cis-2,4-dihydroxypyrrolidin-1-yl)carbonyl]-2-ethylbutanoyl]-O-(2,6-dichlorobenzyl)-L-tyrosine (II). II and N-[2-[(pyrrolidin-1-yl)carbonyl]-2-ethylbutanoyl]-4-(2,6-

L12 ANSWER 66 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

dichlorobenzoylamino)-L-phenylalanine inhibited the binding of human recombinant VCAM-1 to human B lymphoma cell line expressing integrin.alpha.4.beta.7 with IC50 of .ltoreq.0.02 .mu.mol/L.

IT **340717-95-5P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of novel phenylalanine derivs. as .alpha.4-integrin inhibitors)
RN 340717-95-5 CAPLUS
CN L-Phenylalanine, N-[[1-[(dimethylamino)carbonyl]cyclopropyl]carbonyl]-4-[(7aS)-tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3
REFERENCE(S): (1) F Hoffmann-La Roche Ag; EP 1005446 A1 CAPLUS
(2) F Hoffmann-La Roche Ag; WO 9910313 A1 1999 CAPLUS
(3) Merck & Co Inc; WO 0112183 A1 2001 CAPLUS

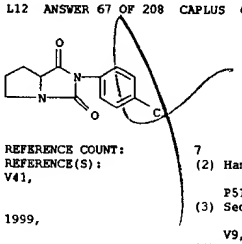
L12 ANSWER 67 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 2000:810729 CAPLUS
DOCUMENT NUMBER: 134:110100
TITLE: Immunomodulator structure-activity relationships: contribution of molecular modeling
AUTHOR(S): Panouse, J. J.; Giorgi, H.; Daspet, J.-P.; Seilles, E.; Robert, J.-F.
CORPORATE SOURCE: Equipe de Chimie therapeurique et Laboratoire de Biophysique medicale et pharmaceutique, Faculte de Medecine et de Pharmacie, Besancon, F 25000, Fr.
SOURCE: Ann. Pharm. Fr. (2000), 58(5), 291-302
CODEN: APFRAD; ISSN: 0003-4509
PUBLISHER: Masson Editeur
DOCUMENT TYPE: Journal
LANGUAGE: French

AB Mol. modeling used to compare 64 immunostimulant compds. with pyrrole quinolein or purine nuclei has pointed out that a common spatial structure is found in most of the active compds. An addnl. study of immunostimulants (levamisole, muramyldipeptide) or immunosuppressive mols. (rapamycin) was performed. A common pharmacophore was found on every studied compd. It was composed of three neighboring electroattractive atoms and a further fourth atom. The favorable conformation of rapamycin for immunosuppressive action, which is not the more stable conformation, could explain the loss of its activity, or those of related macrolides, when some minor chem. modifications are tested. These findings validate the proposed concept and provide a view of the mechanism of action of most of the immunomodulator compds. for prepg. novel compds.

IT **60725-59-9D**, derivs.
RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(mol. modeling and structure-activity relationships for immunomodulators)

RN 60725-59-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-(4-chlorophenyl)tetrahydro- (9CI) (CA INDEX NAME)

L12 ANSWER 67 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



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ALL CITATIONS AVAILABLE IN THE RE FORMAT

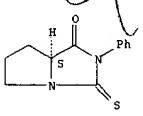
L12 ANSWER 68 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 2000:413023 CAPLUS
DOCUMENT NUMBER: 133:129348
TITLE: Fast separation of amino acid phenylthiohydantoin derivatives by HPLC on a non-porous stationary phase
AUTHOR(S): Boros, B.; Kovacs, K.; Ohmacht, R.
CORPORATE SOURCE: Institute of Medical Chemistry, University Medical School, Pecs, 7624, Hung.
SOURCE: Chromatographia (2000), 51(Suppl.), S202-S204
CODEN: CHRGB7; ISSN: 0009-5893
PUBLISHER: Friedrich Vieweg & Sohn Verlagsgesellschaft mbH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A new method is described for the sepn. of phenylthiohydantoin (PTH) derivs. of the 20 common amino acids. The anal. requires .apprx.7 min and good resoln. was obtained by RP-HPLC on columns packed with a nonporous stationary phase (Kovasil-C14; 33 .times. 4.6 mm). Gradient elution was chosen with eluents contg. either sodium acetate/acetic acid buffers (moderately acidic conditions) or a heptafluorobutyric acid modifier (strongly acidic eluent). A slightly different elution order of the PTH-amino acids was found in the two systems. Low detection limits (in the femtomol range) were achieved with simple com. HPLC equipment.

IT **29635-99-2**
RL: ANT (Analyte); PEP (Physical, engineering or chemical process); ANST (Analytical study); PROC (Process)
(fast sepn. of amino acid phenylthiohydantoin derivs. by HPLC on nonporous stationary phase)

RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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REFERENCE(S):
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L12 ANSWER 68 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
(5) Lottspeich, F; Z Physiol Chem 1980, V361, P1829 CAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

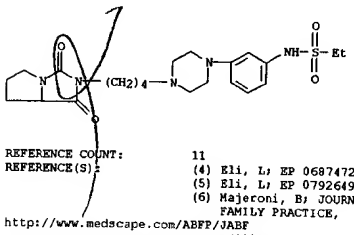
L12 ANSWER 69 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 2000:98327 CAPLUS
DOCUMENT NUMBER: 132:146650
TITLE: Treating depression with a combination of a serotonin uptake inhibitor, a 5-HT1A presynaptic antagonist, and a 5-HT1A agonist
INVENTOR(S): Depoortere, Henri
PATENT ASSIGNEE(S): Sanofi-Synthelabo, Fr.
SOURCE: PCT Int. Appl., 36 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000006160	A1	20000210	WO 1999-FR1825	19990726
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
FR 2781671	A1	20000204	FR 1998-9603	19980728
AU 9949167	A1	20000221	AU 1999-49167	19990726
PRIORITY APPLN. INFO.:			FR 1998-9603 A	19980728
			WO 1999-FR1825 W	19990726

AB Pharmaceutical compns. are provided which contain a serotonin uptake inhibitor (e.g. fluoxetine), a 5-HT1A presynaptic antagonist (e.g. pindolol), and a 5-HT1A agonist (e.g. buspirone) as a combination product for simultaneous, sep., or prolonged use for treating various forms of depression.

IT **221452-76-2**, EF 7412
RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(serotonin uptake inhibitor-5-HT1A presynaptic antagonist-5-HT1A agonist combination for treatment of depression)

L12 ANSWER 69 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
RN 221452-76-2 CAPLUS
CN Ethanesulfonamide, N-[3-[4-[4-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)butyl]-1-piperazinyl]phenyl]- (9CI) (CA INDEX NAME)



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REFERENCE(S):
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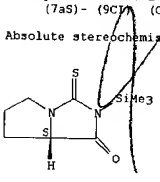
(5) Eli, L; EP 0792649 A 1997 CAPLUS
(6) Majeroni, B; JOURNAL OF THE AMERICAN BOARD OF FAMILY PRACTICE, http://www.medscape.com/ABFP/JABFP/1998/v1 1.n02/fp1102.05.maje/fp1102.05.maje.html abrege 1998, V11(2), P127 MEDLINE
(8) Perez, M; BIOORGANIC & MEDICINAL CHEMISTRY LETTERS 1998, V8(23), P3423 CAPLUS
(9) Puzantian, T; PHARMACOTHERAPY 1999, P205 CAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 70 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1999:661683 CAPLUS
DOCUMENT NUMBER: 132:50225
TITLE: Carboxyl-terminal sequencing: COOH-amino acid activation with DCC or TBTU
AUTHOR(S): Ribeiro, Patricia D.; Alves, Elias W.; Machado, Olga L. T.
CORPORATE SOURCE: Laboratorio de Quimica e Funcao de Proteinas e Peptideos, Centro de Biociencias e Biotecnologia, Universidade Estadual do Norte Fluminense (LQFPP/CBB/UENF), Brazil
SOURCE: Protein Pept. Lett. (1999), 6(4), 203-208
CODEN: PPELEN; ISSN: 0929-8665
PUBLISHER: Bentham Science Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The present study explores conditions to activate the carboxyl group before the coupling of C-terminal amino acid with Trimethylsilyl-isothiocyanate (TMS-ITC). Protected amino acids and different peptides were used as model and 1,3'-Dicyclohexylcarbodiimide (DCC) plus 1-Hydroxybenzotriazole (HOBt) and 2-(1H-Benzotriazol-1-y)-1,1,3,3-tetramethyluronium tetrafluoroborate (TBTU) plus HOBt were used as carboxyl activators. The coupling reaction of activated AA with TMS-ITC was temp. dependent and the best yield (100% of coupling) was obtained at 70.degree.C, when DCC or TBTU both with HOBt were used as activating reagents.

IT **252748-13-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of via amino acid activation with DCC or TBTU in the coupling reaction with trimethylsilyl isothiocyanate for use in carboxyl-terminal sequencing of peptides)
RN 252748-13-3 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-3-thioxo-2-(trimethylsilyl)-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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L12 ANSWER 70 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
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ALL CITATIONS AVAILABLE IN THE RE FORMAT

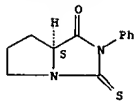
L12 ANSWER 71 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1999:425069 CAPLUS
DOCUMENT NUMBER: 131:211126
TITLE: Separation of phenylthiohydantoin-amino acids by temperature-controlled reversed-phase high-performance liquid chromatography
AUTHOR(S): Hayakawa, Kou; Hirano, Masahiko; Yoshikawa, Kazuyuki; Katsumata, Noriyuki; Tanaka, Toshiaki
CORPORATE SOURCE: Division of Endocrinology and Metabolism, National Children's Medical Research Center, Tokyo, Japan
SOURCE: J. Chromatogr., A (1999), 846(1 + 2), 73-82
CODEN: JCRAEY; ISSN: 0021-9673
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A unique, but general, sepn. method of phenylthiohydantoin (PTH)-amino acids was devised by using a temp.-controlled gradient-elution mode of reversed-phase high-performance liq. chromatog. The gradient was established from two solvents (A* and B*) which consisted of an aq. acidic phosphate buffer soln. (pH 2.1, 0.1 M) and alc. org. modifiers, which afforded stable anal. The column used was Develosil ODS UG-5. The addn. of acetonitrile to solvent B* and running the column at a higher temp. was essential for sepg. PTH-valine and 1,3-diphenyl-2-thiourea. It was found that sepn. of the early-eluting solvophilic amino acids was more efficient at lower column temps., but that a higher temp. was required for sepg. PTH-methionine from PTH-valine, using a 60 A pore diam. ODS silica as model gel. Therefore, temp. control from 35 to 60.degree.C was introduced. Since this sepn. method is reproducible, convenient, and quant., it was applied to the yield anal. of bovine .beta.-lactoglobulin and several peptides after covalent bonding to glass fiber disks.

IT **29635-99-2**
RL: ANT (Analyte); ANST (Analytical study)
(sepn. of phenylthiohydantoin-amino acids by temp.-controlled reversed-phase high-performance liq. chromatog.)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 71 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



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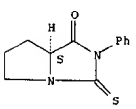
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 72 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1999:96846 CAPLUS
DOCUMENT NUMBER: 130:217292
TITLE: Application of capillary electrochromatography to the separation of phenylthiohydantoin-amino acids
AUTHOR(S): Seifar, Reza M.; Kraak, Johan C.; Poppe, Hans; Kok, Wim Th.
CORPORATE SOURCE: Laboratory for Analytical Chemistry, University of Amsterdam, Amsterdam, 1018 WV, Neth.
SOURCE: J. Chromatogr., A (1999), 832(1 + 2), 133-140
CODEN: JCRAEY; ISSN: 0021-9673
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The applicability of capillary electrochromatog. with 1.5-.mu.m ODS-modified nonporous particles for the sepn. of phenylthiohydantoin (PTH)-amino acids was studied. The effect of the pH, org. solvent content and ion concn. of the mobile phase on the sepn. was studied. On a 34-cm column, plate nos. in the order of 60,000-180,000 were obtained for the neutral and acidic PTH-amino acids. The required presence of sodium dodecyl sulfate (SDS) in the mobile phase led to broad asym. peaks and long retention times for the three basic PTH-amino acids (Arg, His, Lys). With a mobile phase contg. a phosphate buffer with a pH of 7.2, 5 mM SDS, and 5% (vol./vol.) of both acetonitrile and THF, an isocratic sepn. in <8 min could be realized for all PTH-amino acids with the exception of PTH-Arg.

IT **29635-99-2**, PTH-proline
RL: ANT (Analyte); PEP (Physical, engineering or chemical process); ANST (Analytical study); PROC (Process)
(application of capillary electrochromatog. to sepn. of phenylthiohydantoin-amino acids)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 72 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

REFERENCE COUNT: 18
REFERENCE(S):
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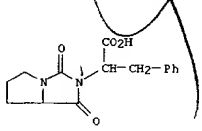
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 73 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1999:36 CAPLUS
DOCUMENT NUMBER: 130:139292
TITLE: Synthesis of hydantoins via N,N'-ureas derived from polymer-bound amino acids
AUTHOR(S): Bauser, M.; Winter, M.; Valenti, C. A.; Wiesmuller, K.-H.; Jung, G.
CORPORATE SOURCE: Institute of Organic Chemistry, University of Tubingen, Tubingen, D-72076, Germany
SOURCE: Mol. Diversity (1998), Volume Date 1997-1998, 3(4), 257-260
CODEN: MODIF4; ISSN: 1381-1991
PUBLISHER: Kluwer Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Starting from carboxy-linked amino acids on trityl functionalized polystyrene resin, a highly efficient solid-phase synthesis of hydantoins via N,N'-ureas was elaborated. The polymer-bound hydantoins can be used as scaffolds for further combinatorial transformations, such as alkylation. Cleavage from the resins yielded the corresponding hydantoins in good yields and purities as shown by ESI-MS and HPLC.
IT **220074-65-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(solid-phase prepn. of hydantoins via N,N'-ureas derived from polymer-bound amino acids)
RN 220074-65-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-2(3H)-acetic acid, tetrahydro-1,3-dioxo-.alpha.-(phenylmethyl)- (9CI) (CA INDEX NAME)



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REFERENCE(S):
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(3) Bhushan, R; J Liq Chromatogr 1987, V10, P3497 CAPLUS
(5) Cunico, R; J Chromatogr 1984, V336, P105 CAPLUS
(6) Edman, P; Acta Chem Scand 1950, V4, P277 CAPLUS
(7) Kim, S; J Chromatogr 1982, V247, P103 CAPLUS
(8) Kulbe, K; Anal Biochem 1971, V44, P548 CAPLUS
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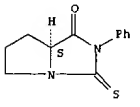
(10) Ware, E; Chem Rev 1950, V46, P403 CAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 74 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1998:787005 CAPLUS
DOCUMENT NUMBER: 130:107063
TITLE: Liquid chromatographic separation of some PTH-amino acids
AUTHOR(S): Bhushan, Ravi; Agarwal, Rachna
CORPORATE SOURCE: Department of Chemistry, University of Roorkee, Roorkee, 247 667, India
SOURCE: Biomed. Chromatogr. (1998), 12(6), 322-325
CODEN: BICHE2; ISSN: 0269-3879
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Liq. chromatog. studies on the sepn. of ten PTH-amino acids were carried out using normal phase untreated silica gel plates, C-18 RP precoated plates and RP-HPLC. Resoln. of a complex mixt. of PTH-amino acids was achieved using all the three types. Certain new successful solvent systems were worked out in each case. HPLC was carried out with Lichrosphere 100 RP-18 (5 .mu.m) column. Acetonitrile and sodium acetate buffer of pH 4.0 was used for reversed phase chromatog. while for normal phase TLC combinations of chloroform-acetonitrile and chloroform-THF were applied.
IT **29635-99-2**, PTH-proline
RL: ANT (Analyte); ANST (Analytical study)
(PTH-amino acids sepn. and identification in mixts. by TLC and HPLC)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)
Absolute stereochemistry.



REFERENCE COUNT: 12
REFERENCE(S):
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(6) Edman, P; Acta Chem Scand 1950, V4, P277 CAPLUS
(7) Kim, S; J Chromatogr 1982, V247, P103 CAPLUS
(8) Kulbe, K; Anal Biochem 1971, V44, P548 CAPLUS

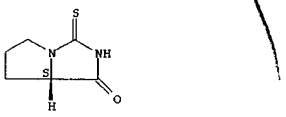
L12 ANSWER 75 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1998:321922 CAPLUS
DOCUMENT NUMBER: 129:65171
TITLE: An efficient and convenient approach to prepare proline thiohydantoin for development of C-terminal sequencing
AUTHOR(S): Mo, Bi-Lan; Li, Jiang; Liang, Song-Ping
CORPORATE SOURCE: Biology Department of Hunan Normal Univ., Changsha, 410081, Peop. Rep. China
SOURCE: Zhongguo Shengwu Huaxue Yu Fenzi Shengwu Xuebao (1998), 14(2), 186-191
CODEN: ZSHXF2; ISSN: 1007-7626
PUBLISHER: Zhongguo Shengwu Huaxue Yu Fenzi Shengwu Xuebao Bianweihui
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

AB A new method to prep. proline thiohydantoin which is required as ref. std. for development of C-terminal sequencing is reported. Proline thiohydantoin was prepd. using a straightforward method involving reaction of proline with trimethylsilylisothiocyanate (TMS-ITC). The product was characterized by amino acid anal., UV spectrum, mass spectrometry and NMR. Different reaction conditions were investigated and the chem. mechanism scheme of proline thiohydantoin is presented. The yield of proline thiohydantoin reached up to 96%.

IT **61160-12-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(an efficient and convenient approach to prep. proline thiohydantoin for development of C-terminal sequencing)

RN 61160-12-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-3-thioxo-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 75 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

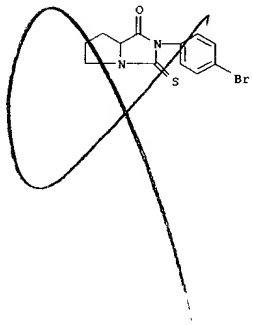
L12 ANSWER 76 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1997:772816 CAPLUS
DOCUMENT NUMBER: 128:58546
TITLE: Molecular shape similarity of cyclic imides and protoporphyrinogen IX
AUTHOR(S): Uraguchi, Ryoichi; Sato, Yukiharu; Nakayama, Akira; Sukekawa, Masayuki; Iwataki, Isao; Boger, Peter; Wakabayashi, Ko
CORPORATE SOURCE: Grad. Sch. Agric. Sci., Tamagawa Univ., Machida, 194, Japan
SOURCE: Nippon Noyaku Gakkaishi (1997), 22(4), 314-320
CODEN: NNGADV; ISSN: 0385-1559
PUBLISHER: Nippon Noyaku Gakkai
DOCUMENT TYPE: Journal
LANGUAGE: English

AB N-Aryl-3,4,5,6-tetrahydrophthalimides, 4-aryl-1,2-tetramethylene-1,2,4-triazolidines, 5-acyl-3,4-tetramethylene-1,3,4-thiadiazolidines, 3-aryl-1,5-tetramethylenehydantoins, and 3-aryl-5-isopropylidene-1,3-oxazolidine-2,4-dione are inhibitors of chlorophyll biosynthesis. The target enzyme is protoporphyrinogen IX oxidase (protox), and these inhibitors interact competitively with the substrate. To est. a steric similarity between cyclic imides and protoporphyrinogen IX (protogen), the most stable mol. structure of these compds. was calcd. and optimized by MOPAC with MNDO-PM3 parameterizations, and their steric properties were compared by computational techniques. For the most stable conformation of cyclic imides, the torsion angles between the imide moiety and benzene ring was approx. 240-270.degree.. By examg. the superimposition patterns, cyclic imides were found to match with the C and D rings of protogen. The 2-carboxyethyl group at the C ring matched with the meta substituent on the benzene ring of the protox inhibitors. The value of the shape similarity index (S) were 0.62-0.85 when protogen and cyclic imides were superimposed by the least square fitting, using the most stable conformation of the protogen mol. A good correlation was found between S and the protox inhibitory index. There is a similarity in the recognition of protox between inhibitors and substructural substrate.

IT **60725-85-1**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); PRP (Properties); BIOL (Biological study); USES (Uses)
(mol. shape similarity of cyclic imides and protoporphyrinogen IX

L12 ANSWER 76 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
studied by MOPAC with MNDO-PM3)

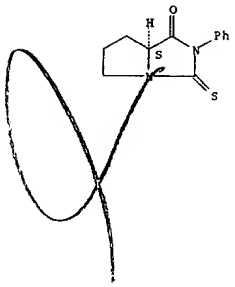
RN 60725-85-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(4-bromophenyl)hexahydro-3-thioxo- (9CI) (CA INDEX NAME)



L12 ANSWER 77 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1997:680964 CAPLUS
DOCUMENT NUMBER: 127:356642
TITLE: High sensitivity analysis of phenylthiohydantoin amino
acid derivatives by electrospray mass spectrometry
AUTHOR(S): Zhou, J.; Hefta, S.; Lee, T. D.
CORPORATE SOURCE: Div. Immunol., Beckman Res. Inst. City Hope, Duare,
CA, 91010, USA
SOURCE: J. Am. Soc. Mass Spectrom. (1997), 8(11), 1165-1174
CODEN: JAMSEF; ISSN: 1044-0305
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A new methodol. has been developed for high sensitivity electrospray ionization mass spectrometric analyses of phenylthiohydantoin (PTH) amino acid derivs. Key components of the methodol. are the use of a solvent system consisting of methanol/dichloromethane (1:1 vol./vol.) contg. 5-mM lithium triflate, a stainless steel electrode having a relatively large surface area, and a microscale electrospray nozzle that provides for stable electrospray at flow rates in the range of 100-500 nL/min. A linear response for the abs. signal intensity of the protonated mol. was obsd. for a no. of derivs. over the concn. range of 50-1000 fmol/.mu.L. For all except the arginine deriv., there was a decrease in the signal intensity with increasing flow rate with 100-300 nL/min being optimum. Collision induced dissocn. (CID) product ion spectra were obtained for 21 derivs. including carboxymethyl cysteine and dehydrothreonine. Leucine and isoleucine can be distinguished on the basis of their CD product ion spectra. A subfentomole detection limit was demonstrated for the phenylalanine PTH deriv. in a selected reaction monitoring (SRM) expt. Samples from an automated Edman microsequence run have been analyzed using the new technique and compared to results obtained by conventional high-performance liq. chromatog. anal. and UV detection. This work demonstrates the feasibility of using mass spectrometry to identify and quantitate the products generated by automated protein microsequencing

L12 ANSWER 77 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
using std. Edman degrdn. chem.
IT **29635-99-2**
RL: ANT (Analyte); ANST (Analytical study)
(high sensitivity anal. of phenylthiohydantoin amino acid derivs. by
electrospray mass spectrometry)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

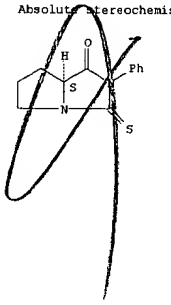
Absolute stereochemistry.



L12 ANSWER 78 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1997:629488 CAPLUS
DOCUMENT NUMBER: 127:274805
TITLE: Capillary Electrochromatography with Gradient Elution
AUTHOR(S): Huber, Christian G.; Choudhary, Gargi; Horvath, Csaba
CORPORATE SOURCE: Institute of Analytical Chemistry and Radiochemistry,
Leopold Franzens University, Innsbruck, 6020, Austria
SOURCE: Anal. Chem. (1997), 69(21), 4429-4436
CODEN: ANCHAM; ISSN: 0003-2700
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A capillary electrochromatograph incorporating a gradient-forming system generally employed in HPLC is described, and the use of gradient elution in reversed phase electrochromatog. is demonstrated by the sepn. of PTH-amino acids and steroid hormones. The gradient former employs 2 reciprocating displacement pumps to control the compn. of the eluent in the reservoir at the column inlet with time in a controlled manner. Thus, the compn. of the mobile phase flowing through the column and driven by electroosmotic forces can be changed with time in a controlled fashion as customary in HPLC with gradient elution. The design of the system allows also for isocratic elution by pumping the eluent of const. compn. through the cavity at the column inlet and thus continuously supplying fresh buffer. The eluent gradient is generated by the 2 pumps and a 10 .mu.L mixer. From there the liq. passes at a flow rate of 0.1-0.2 mL/min through the 17 .mu.L cavity housing the column inlet and an electrode. The flow of the mobile phase was electroosmotic at an effective overall elec. field strength of 500-1500 V/cm through a 50 .mu.m .times. 20/12 cm capillary column packed with 3.5 .mu.m octadecylated silica particles. Gradient profiles generated in this manner were highly reproducible. The same-day and day-to-day reproducibilities of the electroosmotic flow were found to be better than 3%. The use of the capillary electrochromatog. system was demonstrated with isocratic and gradient elution for the sepn. of complex mixts. of biol. interesting substances. The influence of the

L12 ANSWER 78 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
column temp. on the electroosmotic flow velocity and retention of PTH-amino acids was also investigated.
IT **29635-99-2**, PTH-proline
RL: ANT (Analyte); PRP (Properties); ANST (Analytical study)
(capillary electrochromatog. with gradient elution)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

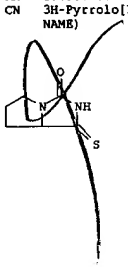


L12 ANSWER 79 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1996:748623 CAPLUS
DOCUMENT NUMBER: 126:16505
TITLE: Method of carboxy terminal protein or peptide sequencing
INVENTOR(S): Anumula, Kalyan Rao
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA; Anumula, Kalyan Rao
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9634289	A1	19961031	WO 1996-US5599	19960418
W: JP, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 5641685	A	19970624	US 1995-427029	19950424
EP 823056	A1	19980211	EP 1996-913030	19960418
R: BE, CH, DE, DK, FR, GB, IT, LI, NL				
JP 11504632	T2	19990427	JP 1996-532637	19960418
US 5968834	A	19991019	US 1996-767122	19961209
PRIORITY APPLN. INFO.:			US 1995-427029	19950424
			WO 1996-US5599	19960418

AB The present invention provides an efficient method for the C-terminal sequencing of proteins or peptides under acidic conditions using acetyl chloride or phosphoryl chloride reacting with a suitable isothiocyanate for derivatization of the carboxy terminus to a thiohydantoin amino acid deriv. Cleavage of the derivatized thiohydantoin amino acid occurs with thiocyanic acid and acetic acid in water and also with the use of a buffer and potassium or sodium thiocyanate or potassium or sodium dithionite reagent. The invention also provides C-terminal sequencing of proteins or peptides by first reacting the peptide or protein with an acid chloride reagent, such as acetyl chloride and with an org. isothiocyanate, an org. salt thiocyanate, or metal thiocyanate to yield a thiohydantoin amino acid deriv. The thiohydantoin amino acid deriv. may be cleaved using either acidic or basic conditions.

L12 ANSWER 79 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
IT **184305-04-2P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(C-terminal protein or peptide sequencing)
RN 184305-04-2 CAPLUS
CN 3H-Pyrrolo[1,2-c]imidazol-3-one, hexahydro-1-thioxo- (9CI) (CA INDEX NAME)



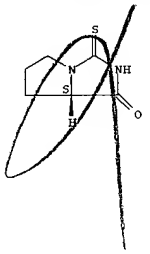
L12 ANSWER 80 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1996:159511 CAPLUS
DOCUMENT NUMBER: 124:225775
TITLE: Automated C-terminal sequencing of polypeptides containing C-terminal proline
AUTHOR(S): Bailey, Jerome M.; Tu, Oanh; Issai, Gilbert; Shively, John E.
CORPORATE SOURCE: Division Immunology, Beckman Research Institute the City Hope, Duarte, CA, 91010, USA
SOURCE: Methods Protein Struct. Anal., [Proc. Int. Conf.], 10th (1995), Meeting Date 1994, 131-8.
Editor(s): Atassi, M. Zouhair; Appella, Ettore. Plenum: New York, N. Y.
CODEN: 62LPAK
DOCUMENT TYPE: Conference
LANGUAGE: English

AB Inglis et al. (1993), using a procedure similar to that described by Kubo et al. (1971), described the successful synthesis of thiohydantoin-proline from N-acetylproline. This was done by the 1-pot reaction of acetic anhydride, HOAc, TFA, and ammonium thiocyanate with N-acetylproline. Here the authors reproduce this synthesis and develop it further into a large-scale synthesis (200 mg) of thiohydantoin-proline. They also describe the development of chem. based on the diphenylphosphoroisothiocyanatidate/pyridine reaction that permits the efficient derivatization and hydrolysis of peptidyl C-terminal proline to a thiohydantoin and discuss the integration of this chem. into an automated method for the C-terminal sequence anal. of polypeptides contg. C-terminal proline.

IT **61160-12-1P**, 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-3-thioxo-, (S)-
RL: SPN (Synthetic preparation); PREP (Preparation)
(automated C-terminal sequencing of polypeptides contg. C-terminal proline)
RN 61160-12-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-3-thioxo-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 80 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



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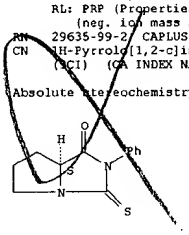
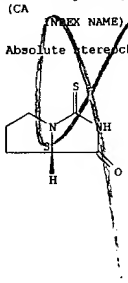
L12 ANSWER 81 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1995:981103 CAPLUS
DOCUMENT NUMBER: 124:176843
TITLE: The negative ion mass spectra of (M-H)- ions from the phenylthiohydantoin derivatives of amino acids
AUTHOR(S): Ramsay, Steven L.; Waugh, Russell J.; Blumenthal, Thomas; Bowie, John H.
CORPORATE SOURCE: Dep. Chem., Univ. Adelaide, 5005, Australia
SOURCE: Eur. Mass Spectrom. (1995), 1(4), 381-7
CODEN: EMSPFW; ISSN: 1356-1049
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The mass spectra of (M-H)- ions of phenylthiohydantoin (PTH) amino acids show characteristic fragmentations through the side chain (the .alpha.-side chain of the original amino acid) which may be used to identify each of the common amino acids. Some of these fragmentations are Leu (C3H8), Ile (CH4, C2H6), Phe (PhH), Tyr (CH2C6H4O), Trp (CH2C8H5N), Ser (CH2O), Thr (MeCHO) and Met (MeSH). The formulas in parentheses represent the neutrals lost.
IT **29635-99-2**, L-Proline phenylthiohydantoin
RL: PRP (Properties)
(neg. ion mass spectra of amino acid phenylthiohydantoin derivs.)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 82 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1995:604208 CAPLUS
DOCUMENT NUMBER: 123:51613
TITLE: C-terminal sequence analysis of polypeptides containing C-terminal proline
AUTHOR(S): Bailey, Jerome M.; Tu, Oanh; Issai, Gilbert; Shively, John E.
CORPORATE SOURCE: Div. Immunol., Beckman Res. Inst. of the City of Hope, Duarte, CA, 91010, USA
SOURCE: Tech. Protein Chem. VI, [Pap. Symp. Protein Soc.], 8th (1995), Meeting Date 1994, 239-47. Editor(s): Crabb, John W.. Academic: San Diego, Calif..
CODEN: 61MDAG
DOCUMENT TYPE: Conference
LANGUAGE: English
AB The thiohydantoin proline synthesis method of A. S. Inglis and C. De Luca (1993) was reproduced and developed into a large scale synthesis. The development of chem. based on the di-Ph phosphoroisothiocyanatidate/pyridine reaction that permits the efficient derivatization and hydrolysis of peptidyl C-terminal proline to a thiohydantoin is described, and the integration of this chem. into an automated method for the C-terminal sequence anal. of proteins contg. C-terminal proline is discussed.
IT **61160-12-1P**
RL: ANT (Analyte); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)
(C-terminal sequence anal. of polypeptides contg. C-terminal proline)
RN 61160-12-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-3-thioxo-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

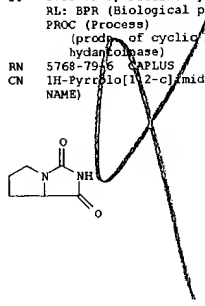


L12 ANSWER 82 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

L12 ANSWER 83 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1995:506335 CAPLUS
DOCUMENT NUMBER: 122:237925
TITLE: Production of cyclic N-carbamoyl-D-amino acids
INVENTOR(S): Bommarius, Andreas; Schaefer, Matthias; Drauz, Karlheinz
PATENT ASSIGNEE(S): Degussa A.-G., Germany
SOURCE: Ger. Offen., 4 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4330678	A1	19950316	DE 1993-4330678	19930910

OTHER SOURCE(S): MARPAT 122:237925
AB A process for the prodn. of cyclic N-carbamoyl-D-amino acids from the corresponding hydantoins with the use of a hydantoinase is disclosed.
IT **5768-79-6**, Proline hydantoin
RL: BPR (Biological process); RCT (Reactant); BIOL (Biological study); PROC (Process)
(prodn. of cyclic N-carbamoyl-D-amino acids from hydantoins using a hydantoinase)
RN 5768-79-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro- (9CI) (CA INDEX NAME)



L12 ANSWER 84 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1995:338919 CAPLUS
DOCUMENT NUMBER: 122:100720
TITLE: Automated carboxy-terminal sequence analysis of polypeptides containing C-terminal proline
AUTHOR(S): Bailey, Jerome M.; Tu, Oanh; Issai, Gilbert; Ha, Alice; Shively, John E.
CORPORATE SOURCE: Beckman Res. Inst. of the City of Hope, Div. Immunology, Duarte, CA, 91010, USA
SOURCE: Anal. Biochem. (1995), 224(2), 588-96
CODEN: ANBCA2; ISSN: 0003-2697
DOCUMENT TYPE: Journal
LANGUAGE: English

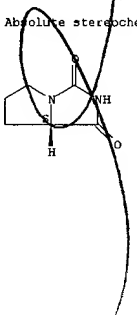
AB Proteins and peptides can be sequenced from the carboxy-terminus with isothiocyanate reagents to produce amino acid thiohydantoin derivs. Previous studies in the lab. have focused on automation of the thiocyanate chem. using di-Ph phosphoroisothiocyanatidate (DPP-ITC) and pyridine to derivatize the C-terminal amino acid to a thiohydantoin and sodium trimethylsilanolate for specific hydrolysis of the derivatized C-terminal amino acid (Bailey, J. M. et al., 1992). A major limitation of this approach was the inability to derivatize C-terminal proline. The authors now describe chem. based on the DPP-ITC/pyridine reaction which is capable of derivatizing C-terminal proline to a thiohydantoin. The reaction of DPP-ITC/pyridine with C-terminal proline rapidly forms an acyl isothiocyanate which is capable of forming a quaternary amine contg. thiohydantoin. Unlike formation of peptidylthiohydantoins with the other 19 commonly occurring amino acids in which cyclization to a thiohydantoin is concomitant with loss of a proton from the amide nitrogen, proline has no amide proton and as a result the newly formed proline thiohydantoin contains an unprotonated ring nitrogen. This cyclic structure if left unprotonated will regenerate C-terminal proline during the cleavage reaction. However, if protonated by the addn. of acid, the proline thiohydantoin ring is stabilized and can be readily hydrolyzed to proline thiohydantoin and a shortened peptide by the addn. of water vapor or alternatively by sodium or potassium trimethylsilanolate, the reagent normally used for the cleavage reaction. By introducing vapor-phase trifluoroacetic acid (TFA) for the protonation reaction and water vapor for the hydrolysis reaction, the authors automated the chem. required for

L12 ANSWER 84 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
derivatization of C-terminal proline. Since the TFA/water steps have no effect on peptidylthiohydantoins formed from the other 19 amino acids, the addnl. steps required for proline were readily integrated into the automated sequencing program, providing for the first time an automated sequencing program which permits the C-terminal sequence anal. of all 20 of the commonly occurring amino acids. Automated programs are described for the C-terminal sequencing of peptides covalently attached to carboxylic acid-modified polyethylene and larger polypeptides noncovalently applied to Zitex (porous Teflon).

IT **40856-87-9P**
RL: ANT (Analyte); SPN (Synthetic preparation); ANST (Analytical study);
PREP (Preparation)
(automated carboxy-terminal sequence detn. of proteins contg. C-terminal proline)

RN 40856-87-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 85 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1994:663670 CAPLUS
DOCUMENT NUMBER: 121:263670
TITLE: Process for the production of calcium salts of hydantoic acids
INVENTOR(S): Bhattacharya, Apurba
PATENT ASSIGNEE(S): Hoechst Celanese Corp., USA
SOURCE: U.S., 5 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

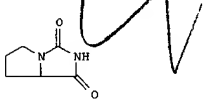
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5338859	A	19940816	US 1993-16628	19930212

OTHER SOURCE(S): MARPAT 121:263670

AB The present invention provides a process for the prodn. of Ca salts of hydantoic acids and which comprises the steps of reacting a hydantoin with a Ca base material such as Ca(OH)2 in an aq. medium to form the Ca salt of the corresponding hydantoic acid and then sepg. the Ca salt of such acid from the reaction mass. This sepn. can include the further steps of cooling the reaction mass down to facilitate the pptn. of the acid/salt crystals and then sepg. the ppt. by means of filtering or centrifugation. These acids can then be subjected to a HNO2-mediated decarbamoylation process followed by an optical resoln. step to thus provide high yields of D-p-hydroxyphenylglycine which is a key synthetic immediate or building block for semi-synthetic pepicillin and cephalosporins.

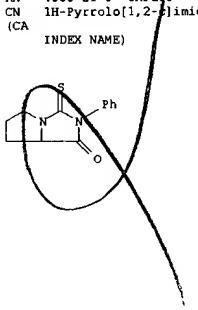
IT **5768-79-6**, 1,5-Trimethylene-hydantoin
RL: RCT (Reactant)
(process for prepn. of hydantoic acid calcium salts with high yields)

RN 5768-79-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro- (9CI) (CA INDEX NAME)



L12 ANSWER 85 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

L12 ANSWER 86 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1994:293258 CAPLUS
DOCUMENT NUMBER: 120:293258
TITLE: Improved thin layer chromatographic resolution of PTH
amino acids with some new solvent systems
AUTHOR(S): Bhushan, R.; Mahesh, V. K.; Varma, A.
CORPORATE SOURCE: Dep. Chem., Univ. Roorkee, Roorkee, 247667, India
SOURCE: Biomed. Chromatogr. (1994), 8(2), 69-72
CODEN: BICHE2; ISSN: 0269-3879
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Three new solvent systems, pyridine-benzene (2.5:20, vol./vol.), methanol-carbon tetrachloride (1:20, vol./vol.) and acetone-dichloromethane (0.3:8, vol./vol.), for the resoln. of a mixt. of 18 PTH amino acids are reported. By using these solvent systems, various combinations of PTH amino acids which had previously posed resoln. problems were resolved and identified.
IT **4333-21-5**, Proline phenylthiohydantoin
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, by TLC, solvents for)
RN 4333-21-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo- (9CI) (CA INDEX NAME)



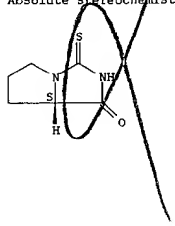
L12 ANSWER 87 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1994:192305 CAPLUS
DOCUMENT NUMBER: 120:192305
TITLE: Method for preparation of amino acid thiohydantoins either in isolation or as the C-terminal of peptides
INVENTOR(S): Inglis, Adam; Tseng, Albert Peng Sheng; Adams, Peter
Laurence
PATENT ASSIGNEE(S): Garvan Institute of Medica Research, Australia
SOURCE: PCT Int. Appl., 33 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9319082	A1	19930930	WO 1993-AU126	19930325
W: AU, CA, JP, KR, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9337412	A1	19931021	AU 1993-37412	19930325
AU 661138	B2	19950713		
EP 635024	A1	19950125	EP 1993-906392	19930325
R: CH, DE, FR, GB, IT, LI, SE				
US 5756667	A	19980526	US 1994-307687	19940923
PRIORITY APPLN. INFO.:			AU 1992-1520	19920325
			AU 1992-4798	19920917
			WO 1993-AU126	19930325

AB The title method involves reacting the amino acid, e.g., proline, or peptide with an acylating agent (e.g., acetic anhydride in acetic acid) and thiocyanate (e.g., ammonium thiocyanate) or isothiocyanate (e.g., guanidine isothiocyanate, trimethylsilyl isothiocyanate, phosphoryl isothiocyanate, and benzoyl isothiocyanate) in the presence of a strong acid (e.g., trifluoroacetic acid, heptafluorobutyric acid, methanesulfonic acid, sulfuric acid, phosphoric acid, and HCl). E.g., proline (or a peptide) is reacted with ammonium thiocyanate, acetic anhydride in acetic acid in the presence of trifluoroacetic acid to give proline thiohydantoin, which was cleaved by trifluoroacetic acid. The tripeptide pyroglutamylleucylprolinamide was analyzed after removal of the amide group with pH 2 formic acid at 110.degree. for 2 h. The result confirmed that proline linked to a leucine did not cleave concomitantly (as does acetylproline), but it did react. This represents a general procedure for

L12 ANSWER 87 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
C-terminal sequencing and may open the door to a combined N- and C-terminal sequencing method for the first time.
IT **61160-12-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cleavage of)
RN 61160-12-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-3-thioxo-, (7aS)- (9CI) (CA INDEX NAME)

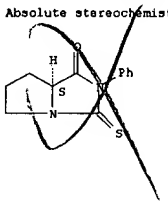
Absolute stereochemistry.



L12 ANSWER 88 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1993:603799 CAPLUS
DOCUMENT NUMBER: 119:203799
TITLE: Edman degradation sequence analysis of resin-bound peptides synthesized by 9-fluorenylmethoxycarbonyl chemistry
AUTHOR(S): Fields, Cynthia G.; VanDrisse, Vickie L.; Fields, Gregg B.
CORPORATE SOURCE: Univ. Minnesota, MN, USA
SOURCE: Pept. Res. (1993), 6(1), 39-47
CODEN: PERREO; ISSN: 1040-5704
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The efficacy of Edman degrdn. sequence anal. for evaluating the synthetic efficiency of peptide-resin assembly by 9-fluorenylmethoxycarbonyl (Fmoc) solid-phase methodol. has been studied. Prior researchers have described the use of solid-phase "preview" sequence anal. for peptides synthesized by tert-butyloxycarbonyl chem., where benzyl-based side-chain protecting groups and peptide-resin linkers are stable to the conditions of Edman chem. The authors have successfully sequenced a variety of resin-bound peptides synthesized by Fmoc chem., where tert-butyl-based side-chain protecting groups and peptide-resin linkers are labile to the conditions of Edman chem. Crude peptides are liberated from trifluoroacetic acid-labile linkers during the first cycle of Edman degrdn. and subsequently "embedded" in membranes. For peptides up to 20 residues, embedded sequencing repetitive yields were comparable to those of solid-phase sequencing. Preview sequencing of resin-bound Fmoc-synthesized peptides proved to be advantageous compared to other anal. methods, in that synthetic failures were detected and quantitated at the point of occurrence, regardless of whether incomplete Fmoc deprotection or incomplete coupling was responsible, and without interference from byproducts formed during peptide-resin cleavage. Quant. ninhydrin anal., which previously has been found to give false pos. results due to removal of the Fmoc group by a combination of reagents and high temp., gave false neg. results in this study, most probably due to incomplete removal of the Fmoc group prior to coupling. Quant. sequence anal. results were supported by high-performance liq. chromatog., amino acid and electrospray mass spectrometric analyses of the crude and purified peptides.
IT **29635-99-2**
RL: ANT (Analyte); ANST (Analytical study)
(high-performance liq. chromatog. of, Edman degrdn. sequence anal. of

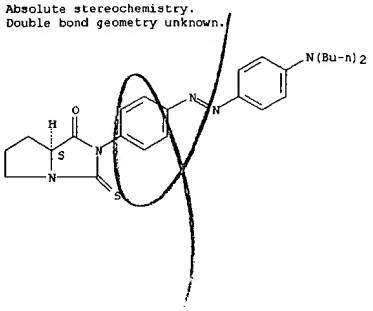
L12 ANSWER 88 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
resin-bound peptides in relation to)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 89 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1993:204429 CAPLUS
DOCUMENT NUMBER: 118:204429
TITLE: Chromatographic separation of some .alpha.-amino acids
in the form of 4-N,N-dibutylaminoazobenzene-4'-thiohydantoin (DBABTH) derivatives
AUTHOR(S): Iskierko, Jerzy; Pyra, Edmund
CORPORATE SOURCE: Dep. Fundam. Chem., Sch. Med., Lublin, 20081, Pol.
SOURCE: Acta Pol. Pharm. (1991), 48(3-4), 9-12
CODEN: APPHAX; ISSN: 0001-6837
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Thiohydantoin derivs. of 15 amino acids RCH(NH2)CO2H (glycine, alanine, leucine, valine, aspartic and glutamic acids, threonine, methionine, arginine, lysine, phenylalanine, tyrosine, tryptophan, proline, and histidine) were prepd. and sepd. by TLC on silica gel using 18 solvent mixts. Only the derivs. of histidine and arginine failed to migrate, whereas those of all other amino acids were resolved and visualized as orange spots (red upon exposure to HCl) with fairly distinct Rf values.
IT **147087-07-8P**
RL: ANST (Analytical study); PREP (Preparation)
(prepn. and thin-layer chromatog. of)
RN 147087-07-8 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-[4-[[4-(dibutylamino)phenyl]azo]phenyl] hexahydro-3-thioxo-, (S)- (9CI) (CA INDEX NAME)

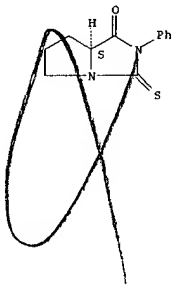
Absolute stereochemistry.
Double bond geometry unknown.



L12 ANSWER 90 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1993:115937 CAPLUS
DOCUMENT NUMBER: 118:115937
TITLE: Detection of liquid injection using an atmospheric pressure ionization radiofrequency plasma source
AUTHOR(S): Zhao, Jianguo; Lubman, David M.
CORPORATE SOURCE: Dep. Chem., Univ. Michigan, Ann Arbor, MI, 48109, USA
SOURCE: Anal. Chem. (1993), 65(7), 866-76
CODEN: ANCHAM; ISSN: 0003-2700
DOCUMENT TYPE: Journal
LANGUAGE: English
AB An atm. pressure rf plasma source which operates in a variety of different buffer gases has been developed as an ionization method for org. samples introduced by liq. injection into atm. pressure ionization mass spectrometry (API/MS). The rf source can operate in He at <1 W of load power at 165 kHz. It can also be sustained in Ar, N2, air, and CO2 at a load power of <15 W. In most cases studied, the protonated mol., MH+, is obsd. with little or no fragmentation even under the relatively high current conditions of the discharge. However, using increasingly higher acceleration voltages between the skimmers in the differentially pumped region between atm. pressure and high vacuum, one can induce fragmentation via collision-induced dissocn. This can be assisted in these expts. via the use of a heavy buffer gas. The detection limits achieved for rf/API plasma detection are typically in the low femtomole region for small org. mols. including neurotransmitters, PTH-amino acids, steroids, drugs, pesticides, and explosives. The detection can be performed with quantitation over at least 4 orders of magnitude.
IT **29635-99-2**, PTH-proline
RL: ANT (Analyte); ANST (Analytical study)
(detection of, by atm. pressure ionization mass spectrometry using radiofrequency plasma source)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 90 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



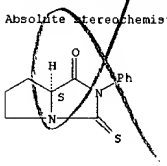
L12 ANSWER 91 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1993:93532 CAPLUS
DOCUMENT NUMBER: 118:93532
TITLE: Effective solvent systems for separation of PTH-amino acids on polyamide sheet
AUTHOR(S): Mustafa, G.; Abbasi, A.; Zaidi, Z. H.
CORPORATE SOURCE: HEJ Res. Inst. Chem., Univ. Karachi, Karachi, 75270, Pak.
SOURCE: Iran. J. Chem. Chem. Eng. (1992), 11(1), 53-6
CODEN: IJCEE9; ISSN: 1011-3509
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Two dimensional thin layer chromatog. on polyamide sheets is a useful method for identification of PTH-amino acids (phenylthiohydantoin-amino acids) which have very close Rf-values. The solvent systems described here are particularly effective and have an edge over other solvent systems used for the sepn. of PTH-amino acids. The solvent systems provide a clear sepn. of all PTH-amino acids except isoleucine/leucine in a relatively short time.

IT **29635-99-2**
RL: ANST (Analytical study); PROC (Process)
(sepn. of, from amino acids by TLC on polyamide sheet, effective solvent systems for)

RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



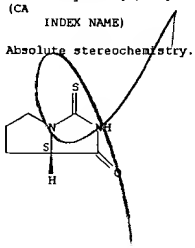
L12 ANSWER 92 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1993:18784 CAPLUS
DOCUMENT NUMBER: 118:18784
TITLE: Formation of proline thiohydantoin with ammonium thiocyanate: progress towards a viable C-terminal amino-acid-sequencing procedure
AUTHOR(S): Inglis, Adam S.; Duncan, Mark W.; Adams, Peter; Tseng, Albert
CORPORATE SOURCE: Garvan Inst. Med. Res., St. Vincent's Hosp., Darlinghurst, 35121, Australia
SOURCE: J. Biochem. Biophys. Methods (1992), 25(2-3), 163-71
CODEN: JBBMDG; ISSN: 0165-022X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Pure amino acid thiohydantoins are required as ref. stds. for development of C-terminal-sequencing procedures based on thiohydantoin formation of the C-terminal amino acids of peptides and proteins. Proline thiohydantoin was prepd. using a straightforward method involving reaction of acetylproline with ammonium thiocyanate. It was characterized by UV spectrophotometry, mass spectrometry and back-hydrolysis to the free amino acid. These data establish unequivocally that the thiocyanate procedure is applicable to profile as well as to the other common amino acids. This work also validates earlier claims that proline thiohydantoin can be prepd. by reaction with thiocyanic acid.

IT **61160-12-1P**
RL: PREP (Preparation)
(prepn. of, as ref. std. for protein sequencing)

RN 61160-12-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-3-thioxo-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



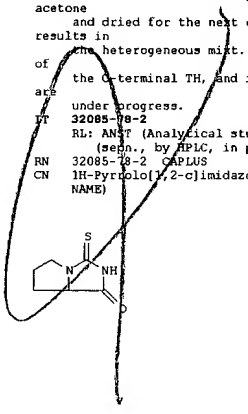
L12 ANSWER 92 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

L12 ANSWER 93 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1992:629357 CAPLUS
DOCUMENT NUMBER: 117:229357
TITLE: Solid-phase C-terminal sequencing of peptides
AUTHOR(S): Goto, M.; Kohara, N.; Yamashita, S.
CORPORATE SOURCE: Dep. Clin. Chem., Hoshi Coll. Pharm., Tokyo, Japan
SOURCE: Amino Acids (1992), 2(3), 289-96
CODEN: AACIE6
DOCUMENT TYPE: Journal
LANGUAGE: English

AB C-terminal amino acid sequence anal. seemed to be an established procedure, as the counterpart of Edman's N-terminal sequencing method. However, poor recovery of the C-terminal amino acids in the reaction in homogeneous soln. suggested further improvement of the method. In the present study, N-terminal amino acid was fixed covalently to controlled pore glass (CPG) beads and the C-terminal amino acid was activated (by treating with acetic anhydride) and coupled with thiocyanate to form a thiohydantoin (TH) ring at the C-terminus. Then, the C-terminal amino acid was split off as the corresponding TH deriv., and analyzed by HPLC. Hydrolysis of the TH deriv. was achieved at 60.degree. in the presence of 2M HCl for 2 h. Solid-phase fixed peptide was washed simply with acetone and dried for the next cycle of the reaction. So far obtained results in the heterogeneous mixt. are not satisfactory in terms of the recovery of the C-terminal TH, and improvement of the recovery and further steps are under progress.

IT **32085-78-2**
RL: ANST (Analytical study)
(sepn., by HPLC, in peptide C-terminal sequencing)

RN 32085-78-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-3-thioxo- (9CI) (CA INDEX NAME)



L12 ANSWER 94 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1992:551304 CAPLUS
DOCUMENT NUMBER: 117:151304
TITLE: Gas-chromatographic determination of methylthiohydantoin amino acid as N(O)-butyldimethylsilyl derivatives in amino acid sequencing with methylisothiocyanate
AUTHOR(S): Woo, Kang Lyung
CORPORATE SOURCE: Dep. Food Eng., Kyungnam Univ., Masan, 631-701, S. Korea
SOURCE: Han'guk Nonghwa Hakhoechi (1992), 35(2), 132-8
CODEN: JKACA7; ISSN: 0368-2897
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Derivatization of amino acids with new silylating reagent Me3CSiMe2NMeCOCF3 (I), instead of the usual N,O-bis(trimethylsilyl)acetamide (II) for the prepn. of trimethylsilyl derivs., was used for effective detn. of methylthiohydantoin amino acids from protein sequencing by GC on HP-1 capillary columns. Twenty one protein amino acids (except cystine) were identified using this method. Arginine, which is not detected by derivatization with II, was resolved with I. Multiple peaks were obsd. in derivatization of Pro, Ile, Gly, Tyr, and esp. hydroxyproline with I. Calibration curves of the derivatized amino acid methylthiohydantions from 2.5 to 7.5 nmol showed good linearity, with Lys, His, and Arg showing linearity from 5.0 to 15.0 nmol. Correlation coeffs. and regression coeffs. of all calibration curves were highly significant (.rho. < 0.001).

IT **1968-34-9**
RL: RCT (Reactant)
(silylation of, with methyl(butyldimethylsilyl)trifluoroacetamide, for anal. by GC)

RN 1968-34-9 CAPLUS

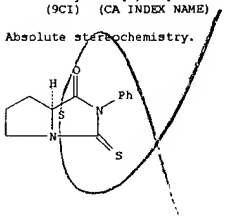
L12 ANSWER 95 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1992:470274 CAPLUS
DOCUMENT NUMBER: 117:70274
TITLE: The development of high-performance liquid chromatographic analysis of allyl and allyloxycarbonyl side-chain-protected phenylthiohydantoin amino acids
AUTHOR(S): Fields, Cynthia G.; Loffet, Albert; Kates, Steven A.; Fields, Gregg B.
CORPORATE SOURCE: Biomed. Eng. Cent., Univ. Minnesota, Minneapolis, MN, 55455, USA
SOURCE: Anal. Biochem. (1992), 203(2), 245-51
CODEN: ANBCA2; ISSN: 0003-2697
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Ten phenylthiohydantoin (PTH) amino acids possessing allyl (Al) or allyloxycarbonyl (Aloc) side-chain-protecting groups have been characterized by HPLC for use in Edman degrdn. sequence anal. Optimized sepn. of side chain-protected and -unprotected PTH amino acids was achieved on a C18 reversed-phase column with a two-step gradient spanning 32 min. Five of the side-chain-protected amino acids [Cys(Al), Cys(Aloc), Lys(Aloc), Thr(Aloc), Tyr(Al)] were completely stable to the conditions of PTH derivatization, four [Asp(OAl), Arg(Aloc)2, Glu(OAl), Ser(Aloc)] were partially deprotected during PTH derivatization, and one [His(Aloc)] was completely deprotected during PTH derivatization. All allyl-based derivs. were well resolved from their side chain-unprotected counterparts. Studies on the stability to piperidine treatment showed Asp(OAl), Cys(Al), Glu(OAl), Lys(Aloc), Thr(Aloc), and Tyr(Al), and possibly Arg(Aloc)2 and Ser(Aloc) were suitable for peptide synthesis by 9-fluorenylmethoxycarbonyl (Fmoc)-based chem. Edman degrdn. of Al and Aloc side-chain-protected Conus geographus Lys9-.alpha.-conotoxin GI synthesized on 4-methylbenzhydrylamine-copoly(styrene-1%-divinylbenzene) resin demonstrated the usefulness of these derivs. for solid-phase preview sequence anal.

IT **29635-99-2**
RL: RCT (Reactant)
(HPLC retention time of)

L12 ANSWER 95 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

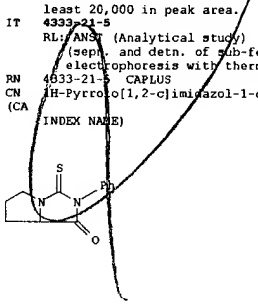


L12 ANSWER 96 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1992:419595 CAPLUS
DOCUMENT NUMBER: 117:19595
TITLE: Sub-femtomole determination of phenylthiohydantoin-amino acids: capillary electrophoresis and thermooptical detection
AUTHOR(S): Waldron, Karen C.; Dovichi, Norman J.
CORPORATE SOURCE: Dep. Chem., Univ. Alberta, Edmonton, AB, T6G 2G2, Can.
SOURCE: Anal. Chem. (1992), 64(13), 1396-9
CODEN: ANCHAM; ISSN: 0003-2700
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Twenty phenylthiohydantion-amino acid acids (PTH-AA) are sepd. by micellar capillary electrophoresis in 13.5 min. A low-energy krypton fluoride laser is used in a thermooptical absorbance detector to produce typical detection limits (3.sigma.) of 9 .times. 10-7M PTH-glycine injected in a 0.6-nL vol., corresponding to 0.5 fmol (100 f) of PTH-glycine injected onto the capillary. Detection limits are roughly 3 orders of magnitude superior to conventional liq. chromatog. detns. Linear dynamic range for this UV absorbance detector is greater than 3000 in peak height and at least 20,000 in peak area.

IT **4333-21-5**
RL: ANST (Analytical study)
(sepn. and detn. of sub-femtomole of, by micellar capillary electrophoresis with thermooptic detection)

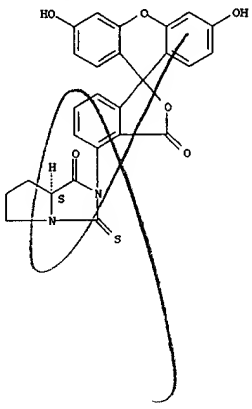
RN 4333-21-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo- (9CI) (CA INDEX NAME)



L12 ANSWER 97 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1992:207099 CAPLUS
DOCUMENT NUMBER: 116:207099
TITLE: Capillary zone electrophoresis separation and laser-induced fluorescence detection of zeptomole quantities of fluorescein thiohydantoin derivatives of amino acids
AUTHOR(S): Wu, Shaole; Dovichi, Norman J.
CORPORATE SOURCE: Dep. Chem., Univ. Alberta, Edmonton, AB, T6G 2G2, Can.
SOURCE: Talanta (1992), 39(2), 173-8
CODEN: TLNTA2; ISSN: 0039-9140
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Capillary zone electrophoresis, when combined with laser-induced fluorescence, is a very powerful technique for the sepn. and detn. of minute amts. of labeled amino acids. This paper presents the detn. of the fluorescein thiohydantoin deriv. of 17 amino acids which takes 13.5 min. The detector, based on laser-induced fluorescence, is optimized with respect to laser power to produce detection limits, three std. deviations above background, ranging from 1 to 2 zeptomoles (1 zeptomole = 1 zmole = 10-21 = 600 analyte mols.) injected into the capillary.
IT **140846-67-9P**
RL: ANST (Analytical study); PREP (Preparation)
(prepn. and capillary zone electrophoresis of, with laser-induced fluorescence detection)
RN 140846-67-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-4-yl)hexahydro-3-thioxo-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

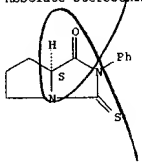
L12 ANSWER 97 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



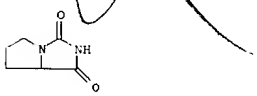
L12 ANSWER 98 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1992:147464 CAPLUS
DOCUMENT NUMBER: 116:147464
TITLE: Evaluation of aminolysis of anilinothiazolinones to phenylthiocarbamoyl amino acid methyl amides as an alternative conversion method in protein sequencing
AUTHOR(S): Pavlik, Manfred; Voburka, Zdenek; Kluh, Ivan; Kostka, Vladimir
CORPORATE SOURCE: Inst. Org. Chem. Biochem., Czech. Acad. Sci., Prague, CS-166 10, Czech.
SOURCE: Anal. Biochem. (1992), 201(1), 9-16
CODEN: ANBCA2; ISSN: 0003-2697
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The aminolysis of products of sequential degrdn. of proteins and peptides by methylamine is an alternative method of conversion of the unstable 5-alkyl-2-anilino-4-thiazolinones into the stable Me amides of N.alpha.-phenylthiocarbamoyl amino acids. The volatility of methylamine permits use in the gas phase during both manual and automatic sequential degrdn. Two procedures were studied: (mode A) aminolysis by methylamine in the sequencer reaction chamber after liberation of the thiazolinones by trifluoroacetic acid and (mode B) aminolysis by methylamine vapors passed through a 1-chlorobutane soln. of thiazolinones in the conversion flask of the sequencer. The sequencing program was modified for both procedures by making use of the std. sequencer functions. The yields of aminolysis in the conversion flask (mode B) are comparable to those obtained by std. conversion in 25% trifluoroacetic acid and the procedure does not affect the repetitive yield. Aminolysis on the glass filter (mode A) requires a major modification of the degrdn. process, yet gives higher yields of the degraded amino acid derivs. A disadvantage of both procedures, esp. of mode A, is the presence of N-methyl-N'-phenylthiourea in the Me amide samples. The expected improvement of the yields of degraded hydroxy amino acids has not been achieved. Therefore the replacement of acid conversion of anilinothiazolinones to phenylthiohydantiones by aminolysis for routine degrdn. cannot be recommended. High yields of Me amides make aminolysis a promising candidate for the incorporation of fluorescent or other labels in the products of sequencing degrdn.
IT **29635-99-2P**
RL: PREP (Preparation)
(prepn. of, in protein sequence detn. using aminolysis by methylamine)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 98 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

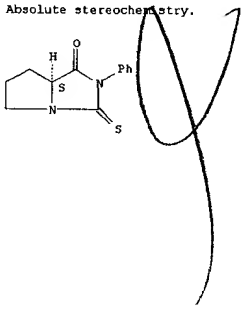


L12 ANSWER 99 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1991:674893 CAPLUS
DOCUMENT NUMBER: 115:274893
TITLE: Determination of amino acid hydantoins by HPLC with diode array detection
AUTHOR(S): Huang, Zhixian; Ough, Cornelius S.
CORPORATE SOURCE: Dep. Vitic. Enol., Univ. California, Davis, CA, 95616, USA
SOURCE: J. Agric. Food Chem. (1991), 39(12), 2218-22
CODEN: JAFCAU; ISSN: 0021-8561
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Eighteen amino acid hydantoins (AAHs) were synthesized from corresponding amino acids and K cyanate. The purity and structure of each hydantoin were confirmed by m.p. measurements and by proton NMR spectroscopy. Some of the AAHs were sepd. by reversed-phase HPLC and detected by a diode array detector at 225 nm. All AAHs tested were sepd. within 15 min with detection limits of 50 pmol. The stability of 12 AAHs was tested, and results indicated that most AAHs were stable in solns. during storage over a period of 6 mo. This method was applied for peptide N-terminal detn. Examples of N-terminal amino acid detn. of 4 peptides are shown.
IT **5768-79-6**, Proline hydantoin
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, by reversed second phase HPLC with diode array detection)
RN 5768-79-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro- (9CI) (CA INDEX NAME)

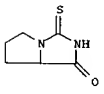


L12 ANSWER 100 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1991:651588 CAPLUS
DOCUMENT NUMBER: 115:251588
TITLE: Analysis of PTH-amino acids with LC/APCI-MS
AUTHOR(S): Uchiyama, Hidefumi; Miura, Kinichiro; Kumagai, Izumi; Takai, Nobuharu
CORPORATE SOURCE: Inst. Ind. Sci., Univ. Tokyo, Tokyo, 106, Japan
SOURCE: Seisan Kenkyu (1991), 43(8), 359-62
CODEN: SKKKAI; ISSN: 0037-105X
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
AB A liq. chromatog./atm. pressure chem. ionization-mass spectrometric method for the detn. of PTH (phenylthiohydantoin)-amino acids is described. This method could det. all PTH-amino acid stds. employed. PTH-asparagine and PTH-histidine, PTH-valine and PTH-proline, and PTH-phenylalanine and PTH-lysine, which were not sepd. by HPLC, could be identified by the mass spectrometry.
IT **29635-99-2**
RL: PROC (Process)
(identification of, by HPLC/atm. pressure chem. ionization mass spectrometry)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

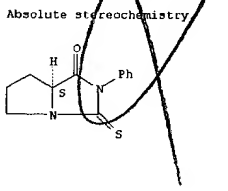


L12 ANSWER 101 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1991:429875 CAPLUS
DOCUMENT NUMBER: 115:29875
TITLE: Microwave irradiation to hydrolyze modified peptide bonds
AUTHOR(S): Yamashita, Saburo; Miyashita, Masahiro; Tsubokawa, Koichiro
CORPORATE SOURCE: Dep. Clin. Chem., Hoshi Coll. Pharm., Tokyo, 142, Japan
SOURCE: Rinsho Kagaku (Nippon Rinsho Kagakkai) (1990), 19(3), 315-21
CODEN: RIKAAN; ISSN: 0370-5633
DOCUMENT TYPE: Journal
LANGUAGE: English
AB For mild and rapid anal. of the C-terminal amino acids of peptides, C-terminal peptide bond was converted to a thiohydantoin ring using $(CF_3CO)_2O$ and thiocyanate and then hydrolyzed by irradiating microwave (2450 MHz) in the presence of 2N HCl for 3 min. The thiohydantoin derivs. of amino acids were sepd. and identified by HPLC. Microwave irradn. was found to be a highly specific method for the hydrolysis of the modified peptide bond.
IT **32085-78-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 32085-78-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-3-thioxo- (9CI) (CA INDEX NAME)



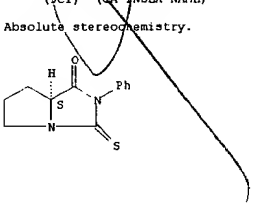
L12 ANSWER 102 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1991:77996 CAPLUS
DOCUMENT NUMBER: 114:77996
TITLE: An optimized procedure for the separation of amino acid phenylthiohydantoins by reversed-phase HPLC
AUTHOR(S): Persson, Bertil; Baker, David
CORPORATE SOURCE: Dep. Biochem., Univ. Uppsala, Uppsala, S-751 23, Swed.
SOURCE: J. Biochem. Biophys. Methods (1990), 21(4), 341-50
CODEN: JBBMDG; ISSN: 0165-022X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB An optimization procedure for the sepn. of 24 phenylthiohydantoin (PTH)-amino acids by HPLC on an inexpensive Merck Superspher Si 60 RP-8 (4.0 .times. 250 mm) column with PTH-norleucine as an internal std. is described. The effects of pH, ionic strength, temp., and gradient were investigated. Using conventional HPLC equipment, the practical detection limit is about 5 pmol.
IT **29635-99-2**
RL: ANT (Analyte); ANST (Analytical study)
(sepn. of, by reversed-phase HPLC)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 103 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1991:35175 CAPLUS
DOCUMENT NUMBER: 114:35175
TITLE: Computer-assisted optimization of separation of PTH-amino acids in HPTLC
AUTHOR(S): Wang, Qinsun; Xie, Wen Qiang
CORPORATE SOURCE: Natl. Lab. Elem. Org. Chem., Nankai Univ., Tianjin, 300071, Peop. Rep. China
SOURCE: J. Planar Chromatogr.--Mod. TLC (1990), 3(March/April), 153-6
CODEN: JPCTE5
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Computer-assisted methods are presented for optimization of single-factor (mobile phase compn.) selection, and for two-factor (mobile phase compn. and impregnate ion concn.) simultaneous selectivity for the optimal sepn. of a series of twelve PTH-amino acids in HPTLC. The 2 methods are based on a statistical technique. The optimization of the expected sepn. response over the exptl. region is based on a special polynomial estd. from preliminary exptl. runs. The Rf difference is used as the selection criterion. Excellent agreement is obtained between predicted and exptl. results for both methods. The two-factor simultaneous selectivity is superior to the single-factor optimization.
IT **29635-99-2**, PTH-proline
RL: ANST (Analytical study)
(sepn. of, single- and two-factor optimization of TLC)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 104 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1991:3043 CAPLUS
DOCUMENT NUMBER: 114:3043
TITLE: Method for preparation of thiohydantoins for carboxyl-terminal protein sequence analysis
INVENTOR(S): Inglis, Adam Sinclair; Casagranda, Franca; Wilshire, John Francis Kelly
PATENT ASSIGNEE(S): Commonwealth Scientific and Industrial Research Organization, Australia
SOURCE: PCT Int. Appl., 23 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

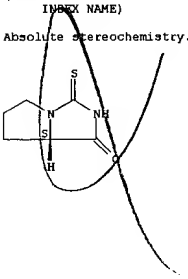
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9004183	A1	19900419	WO 1989-AU433	19891006
W: AU, JP, US				
RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
AU 8944022	A1	19900501	AU 1989-44022	19891006

PRIORITY APPLN. INFO.: AU 1988-840 19881007
AU 1988-939 19881012
WO 1989-AU433 19891006

AB A method for the carboxyl-terminal degrdn. of a protein or peptide comprises: (1) coupling the carboxyl group of the carboxyl-terminal amino acid residue of the protein or peptide with thiocyanic acid or a thiocyanate to form a substituted thiohydantoin deriv., and (2) cleaving the substituted thiohydantoin deriv. with a strong inorg. base (e.g. an alkali metal hydroxide of a concn. of >0.2 M, esp. 0.5 M KOH) in the presence of a water-miscible org. solvent (e.g. MeOH) and an antioxidant (e.g. dithioerythritol or dithiothreitol) to form a shortened protein or peptide and the carboxyl-terminal amino acid thiohydantoin which can be identified for sequencing purposes. Prior to the coupling reaction, the carboxyl group is activated with e.g. Ac2O and AcOH. Shortened protein or peptide formed by the cleavage reaction is subjected to .gtoreq.1 further degrdn. cycles, with each such cycle being followed by identification of the C-terminal amino acid thiohydantoin formed by the cleavage reaction.
A peptide bound on glass beads was degraded by the method. The cleavage

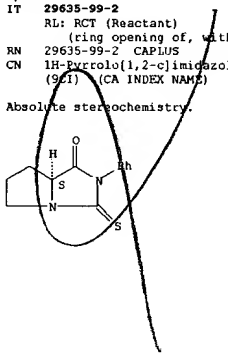
L12 ANSWER 104 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
soln. was analyzed by HPLC. It was possible to sequence through an aspartyl residue, the three successive C-terminal residues (valyl, aspartyl, alanyl) of the peptide being detd. unequivocally. In addn., leucine-enkephalin has been completely sequenced and the synthetic decapeptide (Tyr-Leu-Ala-Ile-Tyr-Val-Met-Ala-Phe-Val) sequenced through to the penultimate residue.
IT **61160-12-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, for protein sequence detn.)
RN 61160-12-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-3-thioxo-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 105 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1990:179770 CAPLUS
DOCUMENT NUMBER: 112:179770
TITLE: Preparation, spectral and physiochemical characteristics of methylamide N.alpha.-phenylthiocarbamoyl derivatives of naturally occurring amino acids
AUTHOR(S): Pavlik, Manfred; Kluh, Ivan; Pavlikova, Frantiska; Vasickova, Sona; Kostka, Vladimir
CORPORATE SOURCE: Inst. Org. Chem. Biochem., Slovak Acad. Sci., Prague, 166 10/6, Czech.
SOURCE: Collect. Czech. Chem. Commun. (1989), 54(7), 1940-54
CODEN: CCCCAK; ISSN: 0010-0765
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:179770
AB Nineteen title derivs. PhNHCS-X-NHMe (X = amino acid residue) were prepd. either by addn. of PhNCS to amino acid methylamides or by treatment of amino acid phenylthiohydantoins with MeNH2. The derivs. were characterized by their m.ps., 1H and 13C NMR, mass, UV, and IR spectra.
IT **29635-99-2**
RL: RCT (Reactant)
(ring opening of, with methylamine)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 106 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1990:32794 CAPLUS
DOCUMENT NUMBER: 112:32794
TITLE: Examination of automated polypeptide sequencing using standard phenylisothiocyanate reagent and subpicomole high-performance liquid chromatographic analysis
AUTHOR(S): Tempst, Paul; Riviere, Lise
CORPORATE SOURCE: Howard Hughes Med. Inst., Harvard Med. Sch., Boston, MA, 02115, USA
SOURCE: Anal. Biochem. (1989), 183(2), 290-300
CODEN: ANBCA2; ISSN: 0003-2697
DOCUMENT TYPE: Journal
LANGUAGE: English

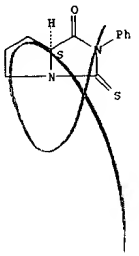
AB The feasibility of accurate protein sequencing at the subpicomole level, using automated Edman chem. and online HPLC anal., was studied. Several modifications of the std. system were first introduced. A larger portion of the phenylthiohydantoin amino acids (70%) is analyzed. Dissoln. in 10% acetonitrile is improved by short periodic bursts of argon. Losses on the column of subpicomole amts. of analytes, in the presence and absence of scavengers, were quantitated; they are related to destruction rather than to unspecific sticking to the stationary phase. Baseline drift, for a large part caused by the presence of UV absorbing N,N-dimethylphenylthiourea in solvent B, is completely eliminated by the addn. of a 2-fold molar excess of tryptophan to solvent A. This allows real time recording of the 269-nm absorption detector signal at 0.0005 absorption unit full scale. The combined modifications result in an 8-fold increase in sensitivity over std. methods. Sequence calling at the 2-10 pmol level, through visual inspection of chromatograms, becomes increasingly simple this way. Once the sequenceable signal drops below the 1 pmol level in the course of a run, meticulous comparison and matching of the preliminary calls with a spreadsheet of peak integration data are necessary for accurate assignments. Reliable sequencing, with signals at the subpicomole level, is now feasible for stretches of over 10 residues. Contaminating amino acids and polypeptides and incompletely

L12 ANSWER 106 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

removed reaction byproducts constitute a major problem for anal. at this level. Future limits to sensitivity of Edman sequencing will primarily depend on improved microprepns. of proteins in cleaner environments, higher purity reagents and solvents, instrument miniaturization, and solid-phase techniques.

IT **29635-99-2**, PTH-Proline
RL: ANT (Analyte); ANST (Analytical study)
(HPLC of, in protein sequencing)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



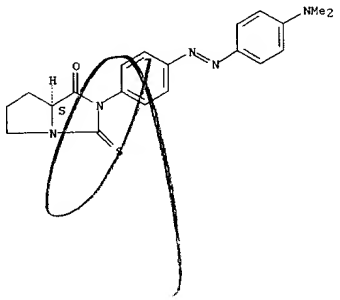
L12 ANSWER 107 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1989:570338 CAPLUS
DOCUMENT NUMBER: 111:170338
TITLE: Improvements in the application of the 4,4-N,N-dimethylaminoazobenzene-4'-isothiocyanate micromethod to the sequence analysis of proteins
AUTHOR(S): Salva, Miquel; Aviles, Francesc X.
CORPORATE SOURCE: Inst. Biol. Fonamental, Univ. Auton. Barcelona, Bellaterra, 08193, Spain
SOURCE: Anal. Biochem. (1989), 180(2), 374-9
CODEN: ANBCA2; ISSN: 0003-2697
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Different exptl. conditions have been tested to improve the sequence detn. of peptides and proteins by the DABITC (4,4-N,N-dimethylaminoazobenzene-4'-isothiocyanate) method and to facilitate automation in the anal. of the released 4,4-N,N-dimethylaminoazobenzene-5'-thiohydantoin derivs. (DABTHs). Conditions for a complete and rapid sepn. of all amino acid derivs. have been optimized by using different reversed-phase columns. The stability of the DABTHs in several water-org. solvent mixts. was detd. by quant. anal. and permitted the selection of the appropriate solvents for use in autosamplers. Also the amino acid side-products specific to individual residues which may be obsd. during thin-layer chromatog. of DABTHs can be completely resolved by HPLC and are helpful for a safe assignment of the amino acid residues. The anal. procedures developed have been used to exam. the influence of O and detergents on the efficiency of the application of the DABITC manual micromethod on proteins. In the presence of O the recovery of DABTHs is lower in most cases than when the operation is carried out in an inert atm. The presence of a limited amt. of detergents does not interfere in the HPLC anal. of DABTHs and, moreover, can increase the efficiency of the sequence anal. of proteins depending on their nature and concn. In particular, it has been obsd. that SDS at a concn. of 0.1% can in some cases produce a 3-fold increase in the recovery of DABTHs.

IT **103697-53-6**
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, by HPLC, optimization of)
RN 103697-53-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-[4-[[4-(dimethylamino)phenyl]azo]phenyl]hexahydro-3-thioxo-, (S)- (9CI) (CA INDEX NAME)

L12 ANSWER 107 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

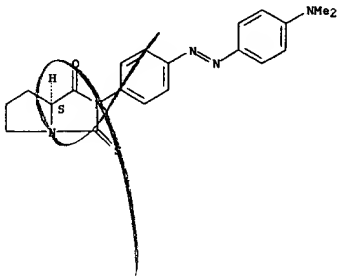
Absolute stereochemistry.
Double bond geometry unknown.



L12 ANSWER 108 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1989:453518 CAPLUS
DOCUMENT NUMBER: 111:53518
TITLE: Analysis of 4-N,N-dimethylaminoazobenzene 4'-thiohydantoin amino acids at sub-picomole levels by high-performance liquid chromatography: simultaneous manual sequencing of picomole quantities of several polypeptides
AUTHOR(S): Fischer, Peter M.; Howden, Merlin E. H.
CORPORATE SOURCE: Div. Biol. Health Sci., Deakin Univ., Geelong, 3217, Australia
SOURCE: Anal. Biochem. (1989), 177(1), 46-9
CODEN: ANBCA2; ISSN: 0003-2697
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A single-column HPLC sepn. of 4-N,N-dimethylaminoazobenzene 4'-thiohydantoin amino acid derivs., generated during polypeptide sequence anal. by the 4-N,N-dimethylaminoazobenzene 4'-isothiocyanate/phenylisothiocyanate double coupling technique, is described. Recovery of the serine and threonine derivs. was improved by substituting BF3-Et2O for trifluoroacetic acid in the thiazolinone cleavage reactions. Residues, including the S-carboxymethyl deriv. of cysteine, were assigned after a single injection and a cycle time of 30 min. Quantities of 4-N,N-dimethylaminoazobenzene 4'-thiohydantoin amino acid derivs. as low as 100 fmol were detected. Interference of sequencing artifacts with residue assignment was avoided. This technique allows simultaneous manual sequencing of several proteins or peptides at the level of a few picomoles.
IT **103697-53-6**
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, by HPLC, in peptide and protein sequencing)
RN 103697-53-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-[4-[[4-(dimethylamino)phenyl]azo]phenyl]hexahydro-3-thioxo-, (S)- (9CI) (CA INDEX NAME)

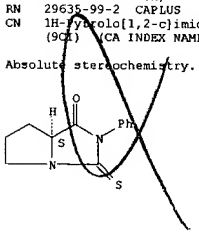
Absolute stereochemistry.
Double bond geometry unknown.

L12 ANSWER 108 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



L12 ANSWER 109 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1989:436190 CAPLUS
DOCUMENT NUMBER: 111:36190
TITLE: Determination of PTH-amino acids using the BAS 200A
AUTHOR(S): Shea, Phil; Jacobs, Wes
CORPORATE SOURCE: Bioanal. Syst., West Lafayette, IN, 47906, USA
SOURCE: Curr. Sep. (1989), 9(1-2), 34
CODEN: CUSEEW; ISSN: 0891-0006
DOCUMENT TYPE: Journal
LANGUAGE: English
AB PTH amino acids, at the picomole level, of proteins and peptides were detected and sepd. by liq. chromatog. with a UV detector.
IT **29635-99-2**, PTH-Proline
RL: ANT (Analyte); ANST (Analytical study)
(detn. and sepn. of, from other PTH amino acids by liq. chromatog. with UV detection)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



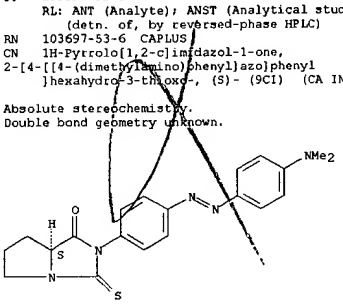
L12 ANSWER 110 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1989:403500 CAPLUS
DOCUMENT NUMBER: 111:3500
TITLE: Reversed-phase high-performance liquid chromatography separation of dimethylaminoazobenzene sulfonyl- and dimethylaminoazobenzene thiohydantoin-amino acid derivatives for amino acid analysis and microsequencing studies at the picomole level
AUTHOR(S): Stocchi, Vilberto; Piccoli, Giovanni; Magnani, Mauro; Palma, Francesco; Biagiarelli, Beatrice; Cucchiarini, Luigi
CORPORATE SOURCE: Ist. Chim. Biol., Univ. Stud. Urbino, Urbino, 61029, Italy
SOURCE: Anal. Biochem. (1989), 178(1), 107-17
CODEN: ANBCA2; ISSN: 0003-2697
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A simple and fast reversed-phase HPLC method has been developed for the complete sepn. of 35 dimethylaminoazobenzene sulfonyl (DABS)-amino acids and byproducts. This method allows simultaneous detn. of primary and secondary amino acids which can be present in protein and peptide hydrolyzates and also detects the presence of cysteic acid, S-sulfocysteine, hydroxyproline, taurine, norleucine, cystine, and .delta.-hydroxylysine. The precolumn derivatization of amino acids with dimethylaminoazobenzene sulfonyl chloride (DABS-Cl) is simple and quick (10 min at 70.degree.) and allows the complete reaction of primary and secondary amino acids. The sepn. of the compds. under investigation is achieved in 25 min using a reversed-phase 3-.mu.m Supelcosil LC-18 column at room temp. The versatility of the proposed method is documented by amino acid detn. on protein samples obtained using different hydrolysis techniques (HCl, methane-sulfonic acid, and NaOH), with attention given to the detection of tryptophan in protein samples with high sugar concn. Furthermore, the exptl. conditions are reported which are necessary to apply this method to the amino acid anal. of very low amt. of proteins (1 to 5 .mu.g) electroeluted from a stained band after sodium dodecyl sulfate-polyacrylamide gel electrophoresis. The stability of DABS-derivs., the short time of anal., the high reproducibility and sensitivity of the system, and the complete resoln. of all compds. of interest make this method suitable for routine anal. Furthermore, a fast reversed-phase HPLC method was developed for the complete sepn. of dimethylaminoazobenzene thiohydantoin (DABTH)-amino acids. The sepn. of

L12 ANSWER 110 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
the compds. under investigation is obtained, at room temp., in less than
18 min using a reversed-phase Supelcosil LC-18 DB column, 3-.mu.m particles, and also allows the complete sepn. of DABTH-isoleucine, DABTH-leucine, and DABTH-norleucine. The short time of anal., together
with the high reproducibility of the system and its sensitivity at picomole levels, make this method very suitable for the identification of
DABTH-amino acids released during microsequencing studies of proteins and
peptides with the dimethylaminoazobenzene isothiocyanate reagent. It is
possible to obtain complete sepn. of DABTH-amino acids also under isocratic conditions. However, in this case, it is necessary to elute the
excess reagent from the column at the end of the day, and this can only be
achieved using a high concn. of solvent B (85% acetonitrile). The 2 different HPLC methods are recommended for amino acid anal. and microsequencing.

IT **103697-53-6**
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, by reversed-phase HPLC)

RN 103697-53-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-[4-[[4-(dimethylamino)phenyl]azo]phenyl]hexahydro-3-thioxo-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



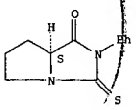
L12 ANSWER 111 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1989:208676 CAPLUS
DOCUMENT NUMBER: 110:208676
TITLE: Isocratic separation of phenylthiohydantoin-amino acids by reversed-phase high-performance liquid chromatography
AUTHOR(S): Hayakawa, Kou; Oizumi, Jun
CORPORATE SOURCE: Div. Metab., Natl. Child. Med. Res. Cent., Tokyo, 154, Japan
SOURCE: J. Chromatogr. (1989), 487(1), 161-6
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English

AB An isocratic system for the simultaneous sepn. of 18 PTH amine acids by
reversed-phase HPLC is described. The HPLC system consisted of a Nucleosil 5-C18 column and a guard column packed with Develosil ODS and
was equipped with a UV (269 nm) detector. Isocratic sepn. was performed
with MeCN-water (40:60) contg. 1% trifluoroacetic acid at a flow rate of
1.0 mL/min. The method is reproducible and has within-day relative std.
deviations for most of the PTH amino acids of 3.1-22%. Results were linear in the range of 0-50 pmol for all the PTH amino acids tested except
for PTH arginine.

IT **29635-99-2**
RL: PROC (Process)
(sepn. of, by isocratic reversed-phase HPLC)

RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



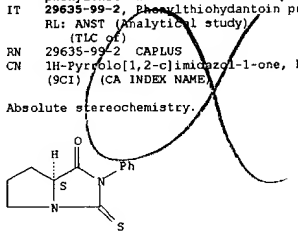
L12 ANSWER 112 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1989:188653 CAPLUS
DOCUMENT NUMBER: 110:188653
TITLE: Improved TLC systems for rapid resolution of phenyl
thiohydantoin amino acids
AUTHOR(S): Bhushan, R.; Mahesh, V. K.; Mallikharjun, P. V.
CORPORATE SOURCE: Dep. Chem., Univ. Roorkee, Roorkee, 247 667, India
SOURCE: Biomed. Chromatogr. (1989), 3(1), 43-5
CODEN: BICHE2; ISSN: 0269-3879
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Two new solvent systems, hexane-propionic acid (26:5) and chloroform-acetone (29:3), for the rapid resoln. and identification of an
18-component mixt. of phenylthiohydantoin amino acids are reported. Using
these systems certain difficult combinations of phenylthiohydantoin amino
acids are resolved. Two more solvent systems, chloroform-acetic acid (27:3) and chloroform-methanol (30:4), are developed to resolve phenylthiodantoin derivs. of aspartic and glutamic acids.

IT **29635-99-2**, Phenylthiohydantoin proline
RL: ANST (Analytical study)
(TLC of)

RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



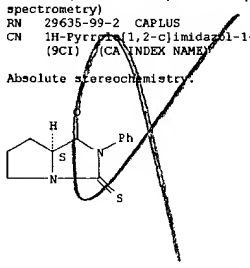
L12 ANSWER 113 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1989:91482 CAPLUS
DOCUMENT NUMBER: 110:91482
TITLE: Peak identification of amino acids in liquid chromatography by optical activity detection
AUTHOR(S): Chan, King C.; Yeung, Edward S.
CORPORATE SOURCE: Ames Lab., USDOE, Ames, IA, 50011, USA
SOURCE: J. Chromatogr. (1988), 457, 421-6
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Phenylthiohydantoin amino acids were detected after chromatog. sepn. using
polarimetric and UV absorption detection. By monitoring both optical activity and UV absorption, the amino acid derivs. that are not identified
by retention times were identified by their optical rotation and vice versa. The detection limits were in the low nanogram range.

IT **29635-99-2**
RL: ANT (Analyte); ANST (Analytical study)
(detection of, after liq. chromatog. by polarimetry or UV spectrometry)

RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 114 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1989:87992 CAPLUS
DOCUMENT NUMBER: 110:87992
TITLE: Structural requirements for hydantoins and 2-thiohydantoins to induce lymphoproliferative popliteal lymph node reactions in the mouse
AUTHOR(S): Kammueller, Michael E.; Seinen, Willem
CORPORATE SOURCE: Fac. Vet. Sci., Univ. Utrecht, Utrecht, 3572 BP, Neth.
SOURCE: Int. J. Immunopharmacol. (1988), 10(8), 997-1010
CODEN: IJIMDS; ISSN: 0192-0561
DOCUMENT TYPE: Journal
LANGUAGE: English

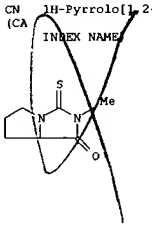
AB The ability of a large no. of hydantoins and 2-thiohydantoins to induce primary local lymphoproliferative popliteal lymph node (PLN) reactions was investigated, as judged by PLN wt. enlargement, in an attempt to evaluate the discriminating potential of the PLN reaction to low-mol.-wt. chems. and to establish structure-activity relationships. Among a series of 19 hydantoins and related compds. only 5,5-diphenylhydantoin (phenytoin), its major metabolite 5-(p-hydroxyphenyl)-5-phenylhydantoin, 5,5-diphenyl-2-thiohydantoin and N-(5-nitro-2-furfurylidene)-1-aminohydantoin (nitrofurantoin) elicited marked PLN reaction in C57BL/6J mice. In DBA/2 mice, PLN responses to the aforementioned compds. were considerably less or virtually absent. A no. of hydantoin derivs. and related compds. with 1 Ph group and(or) other substituents at the 1, 3, or 5 position induced only slightly elevated or suppressed PLN responses in C57BL/6J mice. The influences of polar and lipophilic aliph. and arom. substituents at the 5 position were compared among a series of 22 3-methyl-2-thiohydantoin as well as 21 3-phenyl-2-thiohydantoin amino acid derivs. for their ability to elicit primary PLN reactions in C57BL/6J mice. Substitution with only 1 arom. group at the 5 position seemed to be necessary to induce PLN enlargements by 2-thiohydantoins already substituted at the 3 position with a Me group or even more pronounced when substituted with a Ph group. p-Hydroxylation of 5-benzyl-3-phenyl-2-thiohydantoin diminished the PLN response. In contrast, p-hydroxylation of 1 of 2 Ph groups as in 5-(p-hydroxyphenyl)-5-phenylhydantoin had little

L12 ANSWER 114 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

effect on lymphoproliferative PLN reactions. The presence of an OH group in a nonarom. cyclic substituent as in hexahydro-6-hydroxy-2-methyl-3-thioxo-1H-pyrrolo[1,2-c]imidazol-1-one had no effect on the PLN reaction. Study of a series of aliph. substituents in the 5 position of 2-thiohydantoins showed that the no. of C atoms of the substituents as well as the position of side chains in the isomer, rather than the Me or Ph group in the 3 position of the 2-thiohydantoin mol., detd. the strength of the PLN enlargement. Thus, the PLN wt. increase assay appears to be able to discriminate between subtle chem. differences as studied with a large series of hydantoin and 2-thiohydantoin derivs. The PLN assay may therefore be useful as a preliminary short-term screening method for identification of (classes of) compds. able to induce lymphoproliferative reactions. However, the PLN assay did not identify all hydantoin derivs. and related compds. with documented lymphoproliferative side effects in humans. The possible significance of polymorphisms in drug metab. and disposition, factors not accounted for by the local PLN reaction, is discussed.

IT **22712-58-9**
RL: BIOL (Biological study)
(lymphocyte proliferation stimulation by, structure in relation to)

RN 22712-58-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo- (9CI) (CA INDEX NAME)



L12 ANSWER 115 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1989:54076 CAPLUS
DOCUMENT NUMBER: 110:54076
TITLE: Analysis of phenylthiohydantoin amino acid mixtures for sequencing by thermospray liquid chromatography/mass spectrometry
AUTHOR(S): Pramanik, Bikash C.; Hinton, Stephen M.; Millington, David S.; Dourdeville, Theordore A.; Slaughter, Clive A.
CORPORATE SOURCE: Southwest. Med. Cent., Univ. Texas, Dallas, TX, 75235, USA
SOURCE: Anal. Biochem. (1988), 175(1), 305-18
CODEN: ANBCA2; ISSN: 0003-2697
DOCUMENT TYPE: Journal
LANGUAGE: English

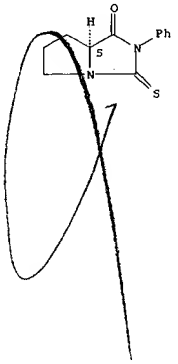
AB Phenylthiohydantoin (PTH) amino acids, the derivs. of amino acids liberated in the course of automated N-terminal sequence anal. of peptides and proteins, are most commonly identified by HPLC. This communication describes an extension to the methodol. for PTH amino acid identification which exploits thermospray liq. chromatog./mass spectrometry for use in the conformation of PTH amino acid identifications previously made solely on the basis of retention times. Thermospray mass spectra of the 19 synthetic PTH amino acids corresponding to the residues commonly obsd. during N-terminal sequencing have been acquired. These spectra show strong signals for the protonated mol. ion, accompanied in several cases by ions produced by limited fragmentation of the amino acid side chain and/or the PTH ring system. A reversed-phase sepn. protocol has been adapted for use with thermospray. The method permits recognition of the protonated mol. ions of all the std. PTH amino acids at the 150-pmol level on the basis of signal-to-noise ratios of 10:1 or better with full scanning. The method has been tested on the N-terminal amino acid sequence anal. of 200 pmol of the std. protein .beta.-lactoglobulin A, and has been found useful in the study of selected side-products of the sequencing chem.

IT **29635-99-2**, Phenylthiohydantoin proline
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, by thermospray liq. chromatog.-mass spectroscopy)

RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)- (9CI) (CA INDEX NAME)

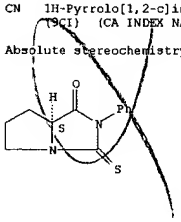
L12 ANSWER 115 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

Absolute stereochemistry.



L12 ANSWER 116 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1989:3919 CAPLUS
DOCUMENT NUMBER: 110:3919
TITLE: Rapid and efficient separation of PTH-amino acids employing supercritical carbon dioxide and an ion pairing agent
AUTHOR(S): Ashraf-Khorassani, M.; Fessahaie, M. G.; Taylor, L.
T.; Berger, T. A.; Deye, J. F.
CORPORATE SOURCE: Dep. Chem., Virginia Polytech. Inst. and State Univ.,
Blacksburg, VA, 24061-0212, USA
SOURCE: HRC CC, J. High Resolut. Chromatogr. Chromatogr. Commun. (1988), 11(4), 352-3
CODEN: HCJCDB; ISSN: 0344-7138
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The supercrit. fluid chromatog. sepn. of phenylthiohydantoin (PTH) derivs.
of amino acids by using a mobile phase gradient of supercrit. CO2 and MeOH
contg. Me4NOH is described. A Zorbax cyanopropyl stationary phase and a
variable wavelength UV detector were used.
IT **29635-99-2**, Phenylthiohydantoin proline
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, by supercrit.-fluid chromatog.)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

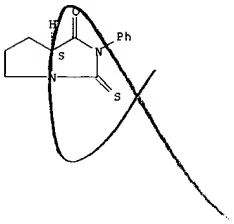
Absolute stereochemistry.



L12 ANSWER 117 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1988:489070 CAPLUS
DOCUMENT NUMBER: 109:89070
TITLE: TLC of phenylthiohydantoin amino acids on silica gel
layers impregnated with metal salts
AUTHOR(S): Bhushan, R.; Reddy, G. P.
CORPORATE SOURCE: Dep. Chem., Univ. Roorkee, Roorkee, 247 667, India
SOURCE: Anal. Lett. (1988), 21(6), 1075-84
CODEN: ANALBP; ISSN: 0003-2719
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The TLC sepn. and identification of PTH-amino acids in a fifteen component
mixt. was reported. TLC plates (20.times.20 cm .times. 0.5 mm) were prepd. by spreading slurries of silica gel impregnated with sulfate, acetate, phosphate, and chloride of zinc; and sulfates of Mg, Mn, Fe, Cd,
and Co. The chromatograms were developed in pre-equilibrated, rectangular
glass chambers using several binary and ternary solvent systems. The spots were located by exposing the chromatograms to iodine vapor. The PTH-amino acids being weak bases, combine with proton and finally form pairs with available anions (like Cl-, SO42-, CH3COO-) and the soly. and
adsorption of the ion pair affects the chromatog. behavior. The methods
are reproducible, simple, require less time, and offer resoln. of several
difficult combinations. The spots are very compact and Rf can be measured
very correctly, for identification purpose, in comparison to iodine-azide
method where bleached spots with diffused boundaries on a light brown background are located. Attempts were also made to det. the partition coeffs. and correlate them with hRf values.
IT **29635-99-2**, PTH-Proline
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, by TLC on silica gels impregnated with metal salts)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

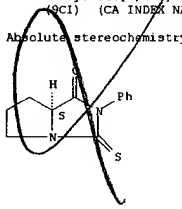
Absolute stereochemistry.

L12 ANSWER 117 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



L12 ANSWER 118 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1988:469689 CAPLUS
DOCUMENT NUMBER: 109:69689
TITLE: Comparison of reverse-phase high-performance liquid
chromatographic methods for precolumn-derivatized amino acids
AUTHOR(S): McClung, G.; Frankenberger, W. T., Jr.
CORPORATE SOURCE: Dep. Soil Environ. Sci., Univ. California, Riverside,
CA, 92521, USA
SOURCE: J. Liq. Chromatogr. (1988), 11(3), 613-46
CODEN: JLCHD8; ISSN: 0148-3919
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A comparison was made among 5 precolumn derivatization techniques for amino acid anal. using reversed-phase HPLC. All chromatog. analyses were
conducted using the same instrumentation and a C18 Ultrasphere ODS column
(5 .mu.m, 250 .times. 4.6 mm). The precolumn derivatization methodologies
studied included the formation of o-phthaldialdehyde, dimethylaminonaphthalenesulfonyl, dimethylaminoazobenzenesulfony, phenylthiohydantoin, and phenylthiocarbamyl derivs. The derivatization
procedures were evaluated for simplicity, time required, and deriv. stability. HPLC analyses of the amino acid derivs. were compared in terms
of resoln., sensitivity, reproducibility, and time of anal.
IT **29635-99-2**, Phenylthiohydantoin proline
RL: ANST (Analytical study)
(chromatog. of, reversed-phase high-performance liq.)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

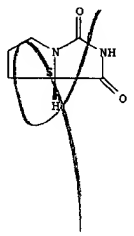
Absolute stereochemistry.



L12 ANSWER 119 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1988:447912 CAPLUS
DOCUMENT NUMBER: 109:47912
TITLE: Decomposition of N-(2-chloroethyl)-N-nitrosocarbamoyl amino acid amides
AUTHOR(S): Suli-Vargha, Helga; Bodi, Jozsef; Meszaros, Miomir; Medzihradszky, Kalman
CORPORATE SOURCE: Res. Group Pept. Chem., Hung. Acad. Sci., Budapest, H-1088, Hung.
SOURCE: J. Med. Chem. (1988), 31(8), 1492-5
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The aq. decompn. of N-(2-chloroethyl)-N-nitrosocarbamoyl-prolinamide (I) and -valinamide (II) were studied under physiol. conditions (0.1 M phosphate buffer at pH 7.4 and 37.degree.). The volatile products were identified by gas chromatog. I gave twice the amt. of ethylene glycol and only 1/5 of the 2-chloroethanol produced by II of the ref. std. BCNU, pointing to different pathways of their decompn. The carbamoylating activity was also investigated in the presence of cyclohexylamine, and it was found to lead mainly to intramol. carbamoylation with the formation of hydantoin derivs. The results are discussed in relation to the antitumor activity of these drugs.
IT **40856-87-9**
RL: BIOL (Biological study)
(as (chloroethyl)nitrosocarbamoylprolinamide carbamoylation product with cyclohexylamine)
RN 40856-87-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-, (7aS)- (9CI) (CA INDEX NAME)

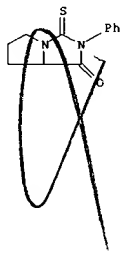
Absolute stereochemistry.

L12 ANSWER 119 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



L12 ANSWER 120 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1988:127806 CAPLUS
DOCUMENT NUMBER: 108:127806
TITLE: On the use of polyethylenimine as a carrier for protein sequencing: comparison with polybrene
AUTHOR(S): Le Caer, Jean Pierre; Rossier, Jean
CORPORATE SOURCE: Lab. Physiol. Nerveuse, Cent. Natl. Rech. Sci., Gif-sur-Yvette, 91198, Fr.
SOURCE: Anal. Biochem. (1988), 169(2), 246-52
CODEN: ANBCA2; ISSN: 0003-2697
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In the gas-liq. phase automated protein sequencer, polyethylenimine was used as a hydrophilic entrapping polymer. Glass fiber filters soaked in a 0.3% soln. of polyethylenimine were used. Sperm whale myoglobin, .beta.-lactoglobulin, and several peptides with basic or acidic pI were sequenced. Loads of 20-26,000 pmol were tested. Initial and repetitive yields compare favorably to those obtained with polybrene-coated glass fiber filters. Recovery of individual amino acids shows that none gave a particularly low yield, in contrast with the low recovery of arginine, tryptophan, histidine, glutamic acid, and aspartic acid when polybrene was used. The usual artifacts were greatly diminished and even disappeared as in the case of N,N'-diphenylurea. Substitution of polyethylenimine for polybrene sped up the anal. because the precycling employed to condition polybrene-coated glass fiber filters was no longer necessary. Polyethylenimine appears superior to polybrene for sequencing proteins and peptides.
IT **4333-21-5**, Proline phenylthiohydantoin
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, by gas-liq. phase automated sequencer, polyethylenimine as carrier in, polybrene comparison with)
RN 4333-21-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo- (9CI) (CA INDEX NAME)

L12 ANSWER 120 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



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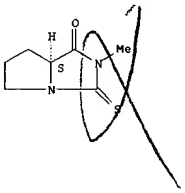
L12 ANSWER 121 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1988:37078 CAPLUS
DOCUMENT NUMBER: 108:37078
TITLE: A natural abundance oxygen-17 NMR investigation of substituted 1-methyl and 1-phenyl-2-thiohydantoins
AUTHOR(S): Boykin, David W.
CORPORATE SOURCE: Dep. Chem., Georgia State Univ., Atlanta, GA, 30303, USA
SOURCE: Heterocycles (1987), 26(3), 773-6
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Natural abundance 17O NMR spectroscopic data for seventeen 1-methyl- and 1-phenyl-2-thiohydantoins obtained in acetonitrile are reported: the relationship of 17O chem. shift to structure is discussed.

IT **28868-23-7**
RL: PRP (Properties)
(oxygen-17 NMR of)

RN 28868-23-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



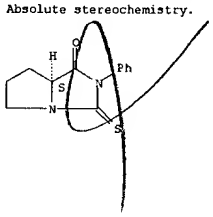
L12 ANSWER 122 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1987:598894 CAPLUS
DOCUMENT NUMBER: 107:198894
TITLE: Analysis of free- and PTH-amino acids by HPLC/MS [high performance liquid chromatography/mass spectrometry] with self-spouting and vacuum nebulizing assisted interface
AUTHOR(S): Matsumoto, Kozo; Tsuge, Shin
CORPORATE SOURCE: Fac. Eng., Nagoya Univ., Nagoya, 464, Japan
SOURCE: Shitsuryo Bunseki (1986), 34(4), 243-8
CODEN: SHIBAK; ISSN: 0542-8645
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The title HPLC/MS system was used to measure the chem. ionization (CI) mass spectra of free- and PTH-amino acids. An aliquot of the injected sample soln. was carried to the interface by a mobile phase (100 .mu.L/min), nebulized under a reduced pressure, and introduced into an ion source where the vapor of the mobile phase was used as a reagent gas for CI. The CI mass spectra of twenty free amino acids were measured using water as mobile-phase. The mass spectra of fifteen PTH-amino acids which eluted successively from a sepn. column were also obtained using a mixt. of acetonitrile and water (3:1 vol. ratio) as mobile phase.

IT **29635-99-2**
RL: PRP (Properties)
(chem.-ionization mass spectra of, high-performance liq. chromatog. system for detn. of)

RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)- (9CI) (CA INDEX NAME)

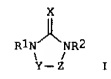
Absolute stereochemistry.



L12 ANSWER 123 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1987:491913 CAPLUS
DOCUMENT NUMBER: 107:91913
TITLE: Cyclic urea derivatives as herbicidal synergists
INVENTOR(S): Lunkenheimer, Winfried; Marzolph, Gerhard; Widdig, Arno; Fedtke, Carl
PATENT ASSIGNEE(S): Bayer A.-G. , Fed. Rep. Ger.
SOURCE: Ger. Offen., 19 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3540919	A1	19870521	DE 1985-3540919	19851119

GI



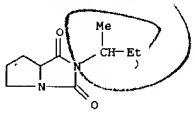
I

AB The cyclic urea deriv. I [R1 = H, alkyl; R2 = alkyl, (un)substituted cycloalkyl, Ph, phenylalkyl; X = O, S; YZ = CH2CO, COCO, COCR3R4, N:CH, C(:CHNMe2)CO, CH2CH2CH2; R3, R4 = H, alkyl] are prepd. as synergists for photosynthesis-inhibiting fungicides. Cyclohexyl isocyanate was added to a cooled mixt. of glycine, NaOH and Me2CO, to give 5-cyclohexylhydantoic acid, which upon refluxing with concd. HCl in EtOH gave I (R1 = H, R2 = cyclohexyl, X = O, YZ = CH2CO) (II). Pre-emergence application of 2 kg II plus 0.1 kg metribuzin/ha gave 80% control of Ipomoea hederacea, whereas the components by themselves were much less effective.

IT **109902-37-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as synergist for photosynthesis-inhibiting herbicides)

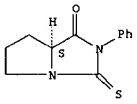
RN 109902-37-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-(1-methylpropyl)- (9CI) (CA INDEX NAME)

L12 ANSWER 123 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

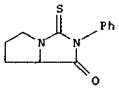


L12 ANSWER 124 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1987:473582 CAPLUS
DOCUMENT NUMBER: 107:73582
TITLE: Retention behavior of phenylthiohydantoin amino acids
in micro high-performance liquid chromatography with
octadecyl bonded glasses and silicas
AUTHOR(S): Okamoto, Mitsuyoshi; Jinno, Kiyokatsu; Yamagami, Mamoru; Nobuhara, Kazunori; Fukushima, Koichi
CORPORATE SOURCE: Gifu Prefect. Tajimi Hosp., Tajimi, 507, Japan
SOURCE: J. Chromatogr. (1987), 396, 345-9
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Four types of octadecyl-modified glasses or silicas were evaluated for
HPLC of 20 typical phenylthiohydantoin amino acids. The amino acids were
sepd. on the glasses as well as the silicas studied, but with different
degrees of resoln. and elution orders.
IT **29635-99-2**, Phenylthiohydantoin proline
RL: ANT (Analyte); ANST (Analytical study)
(chromatog. of, reversed-phase high-performance liq., on octadecyl-bonded glasses and silica)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



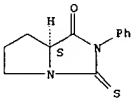
L12 ANSWER 125 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1987:403517 CAPLUS
DOCUMENT NUMBER: 107:3517
TITLE: Rapid resolution of phenylthiohydantoin amino acids by
thin-layer chromatography on silica gel plates impregnated with transition metal ions
AUTHOR(S): Bhushan, R.; Reddy, G. P.
CORPORATE SOURCE: Dep. Chem., Univ. Roorkee, Roorkee, 247667, India
SOURCE: Anal. Biochem. (1987), 162(2), 427-9
CODEN: ANBCA2; ISSN: 0003-2697
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The resoln. of a 15-component mixt. of phenylthiohydantoin (PTH) amino acids using metal ion impregnated silica gel plates is reported. The spots are located by exposing the chromatograms to an I chamber. The method provides a rapid, simple, and less expensive chromatog. system, provides resoln. for certain difficult combinations, and leaves the PTH
amino acids unaltered chem.
IT **4333-21-5**, Proline phenylthiohydantoin
RL: PROC (Process)
(sepn. of, by TLC on transition metal-impregnated silica gel)
RN 4333-21-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo- (9CI) (CA INDEX NAME)



L12 ANSWER 126 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1987:95341 CAPLUS
DOCUMENT NUMBER: 106:95341
TITLE: Determination of phenylthiohydantoin-amino acids by
two-step laser desorption/multiphoton ionization
AUTHOR(S): Engelke, Friedrich; Hahn, Jong Hoon; Henke, Wolfgang;
Zare, Richard N.
CORPORATE SOURCE: Dep. Chem., Stanford Univ., Stanford, CA, 94305, USA
SOURCE: Anal. Chem. (1987), 59(6), 909-12
CODEN: ANCHAM; ISSN: 0003-2700
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The 20 primary phenylthiohydantoin (PTH)-amino acids can be detected and
quantitated by time-of-flight (TOF) mass spectrometry using a 2-step laser
methodol. First a CO2 laser pulse desorbs the PTH-amino acid or a mixt.
thereof prepd. as a thin film on the inside wall of a rotating glass cup.
The latter is part of the 1st electrode of the TOF app. The desorption
process is essentially complete in the laser spot area. After a suitable
time delay, a second UV laser pulse (266 nm) causes 1 + 1
resonance-enhanced multiphonon ionization of the neutral cloud of desorbed
mols. The mass spectra obtained are dominated by the parent ion peak in
almost all cases. Knowledge of the velocity distribution permits flux
measurement. The ion signal is linear in PTH-amino acid concn. in the
range of picomoles to nanomoles. This is the 1st demonstration of quant.
detn. of mols. by laser desorption/multiphoton ionization.
IT **29635-99-2**, Phenylthiohydantoinproline
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, by 2-step laser-desorption/multiphoton-ionization time-of-flight mass spectrometry)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

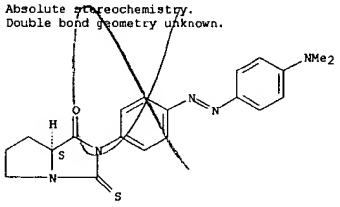
Absolute stereochemistry.

L12 ANSWER 126 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



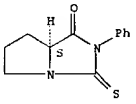
L12 ANSWER 127 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1986:479317 CAPLUS
DOCUMENT NUMBER: 105:79317
TITLE: Complete high-performance liquid chromatographic separation of 4-N,N-dimethylaminoazobenzene-4'-thiohydantoin and 4-dimethylaminoazobenzene-4'-sulfonyl chloride amino acids utilizing the same reversed-phase column at room temperature
AUTHOR(S): Stocchi, Vilberto; Cucchiarini, Luigi; Piccoli, Giovanni; Magnani, Mauro
CORPORATE SOURCE: Ist. Chim. Biol., Univ. Urbino, Urbino, Italy
SOURCE: J. Chromatogr. (1985), 349(1), 77-82
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Reversed-phase high-performance liq. chromatog. methods for the complete
sepn. of title amino acid derivs. on the same Supelcosil LC-18 column at
room temp. are described. The procedures are simple and reproducible, and
the systems are easily interconvertible. The use of a fixed-wavelength
detector at 436 nm permits amino acid anal. at levels lower than 1 pmol
with a stable baseline.
IT **103697-53-6**
RL: PROC (Process)
(sepn. of, by reversed-phase high-performance liq. chromatog.)
RN 103697-53-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-[4-[[4-(dimethylamino)phenyl]azo]phenyl]hexahydro-3-thioxo-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



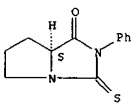
L12 ANSWER 128 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1986:403032 CAPLUS
DOCUMENT NUMBER: 105:3032
TITLE: Pharmaceutical analysis using thermospray liquid chromatography/mass spectrometry and mass spectrometry/mass spectrometry
AUTHOR(S): Unger, Steve E.; Warrack, Bethanne M.
CORPORATE SOURCE: Mass Spectromet. Cent., Squibb Inst. Med. Res., Princeton, NJ, 08540, USA
SOURCE: Spectroscopy (Springfield, Oreg.) (1986), 1(3), 33-8
CODEN: SPECET
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The anal. of phenylthiohydantoin-amino acids and dipeptides using thermospray liq. chromatog./mass spectrometry and mass spectrometry/mass
spectrometry (MS/MS) yields a sensitive and specific method for the rapid
sequencing of small peptides. Beta-lactam antibiotics produce informative
pos. and neg. thermospray mass spectra, and extensive fragmentation is evident in the MS/MS spectra of cephalosporins and penicillins. Monobactams yield numerous degrdn. products in their thermospray spectra.
Thermospray mass spectra of steroids exhibit both mol. wt. and some limited structural information at nanogram levels. MS/MS spectra of steroid sulfoxides resemble electron ionization mass spectra because of
the extensive fragmentation of the steroid nucleus.
IT **29635-99-2**
RL: PROC (Process)
(identification of, by HPLC and mass spectroscopy)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



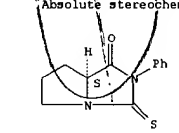
L12 ANSWER 129 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1986:402954 CAPLUS
DOCUMENT NUMBER: 105:2954
TITLE: Separation of phenylthiohydantoin-amino acids by fast
protein liquid chromatography
AUTHOR(S): Johansson, Bo Lennart; Isaksson, Karin
CORPORATE SOURCE: Dep. Qual. Control, Pharm. Biotechnol., Uppsala, S-751
82/1, Swed.
SOURCE: J. Chromatogr. (1986), 356(3), 383-92
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB An optimization strategy for the sepn. of 22 phenylthiohydantoin (PTH)-amino acids is described. The sepn. parameters systematically investigated were the ionic strength, pH, type of org. solvent, column
temp., gradient shape and addn. of different ion-pairing agents. Two different sepn. systems for 2 different column packing materials, PepRPC
and ProRPC, were developed. Reproducibility and detection limits are reported.
IT **29635-99-2**
RL: ANT (Analyte); ANST (Analytical study)
(chromatog. of, fast-protein liq.)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



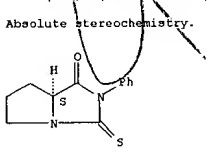
L12 ANSWER 130 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1986:149373 CAPLUS
DOCUMENT NUMBER: 104:149373
TITLE: Separation of phenylthiohydantoin-amino acids in high-performance liquid chromatography and some applications in dansyl Edman sequence analysis
AUTHOR(S): Simmaco, Maurizio; Barra, Donatella; Bossa, Francesco
CORPORATE SOURCE: Ist. Chim. Biol., Univ. "La Sapienza", Rome, Italy
SOURCE: J. Chromatogr. (1985), 349(1), 99-103
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Phenylthiohydantoin (PTH) amino acids were sepd. by high-performance liq.
chromatog. (HPLC). HPLC was applied to the identification of PTH amino
acids recovered in the course of the dansyl Edman degrdn. of a peptide from cytosolic serine hydroxymethyltransferase.
IT **29635-99-2**
RL: ANT (Analyte); ANST (Analytical study)
(high-performance liq. chromatog. of)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



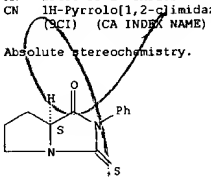
L12 ANSWER 131 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1985:519116 CAPLUS
DOCUMENT NUMBER: 103:119116
TITLE: Microscale isocratic separation of phenylthiohydantoin amino acid derivatives
AUTHOR(S): Lottspeich, Friedrich
CORPORATE SOURCE: Max-Planck Inst. Biochem., Martinsried, D-8033, Fed. Rep. Ger.
SOURCE: J. Chromatogr. (1985), 326, 321-7
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The isocratic sepn. of the common phenylthiohydantoin amino acid derivs. on two columns, suitable for routine analyses, is described. In microsequencing, identification and quantification of the phenylthiohydantoin amino acids at the femtomole level is necessary. With normal anal. columns the detection limit is about 4 pmol. Therefore, microbore columns were used. With the usual equipment, the 2 mm I.D. columns seem to be most effective for the highly sensitive and reliable identification of the phenylthiohydantoin amino acid derivs.
IT **29635-99-2P**
RL: PREP (Preparation)
(prepn. of)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

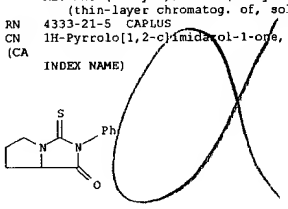


L12 ANSWER 132 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1985:467797 CAPLUS
DOCUMENT NUMBER: 103:67797
TITLE: High-performance liquid chromatography-mass spectrometry of derivatized and underivatized amino acids
AUTHOR(S): Games, David E.; Ramsey, Edward D.
CORPORATE SOURCE: Dep. Chem., Univ. Coll., Cardiff, CF1 1XL, UK
SOURCE: J. Chromatogr. (1985), 323(1), 67-79
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A mixt. of 6 arom. amino acids was studied by moving belt liq. chromatog.-mass spectrometry (LC-MS) using both conventional and microbore columns and by thermospray LC-MS using conventional columns. Microbore columns gave the best detection limits with the moving belt interface. Thermospray LC-MS provides better sensitivity, but 1 of the amino acids was not detected. Methodol. for the direct use of a gradient system with thermospray LC-MS has been developed. Eleven phenylthiohydantoin-amino acids were also studied using a moving belt interface. With microbore columns, detection limits for full scan electron impact spectra ranged 2 nmol-20 pmol.
IT **29635-99-2**
RL: PRP (Properties)
(mass spectrum of)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

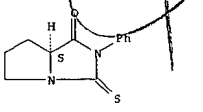


L12 ANSWER 133 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1985:162426 CAPLUS
DOCUMENT NUMBER: 102:162426
TITLE: Amino-terminal sequence analysis of arachin
AUTHOR(S): Bhushan, R.; Goyal, R. N.; Agarwal, Anita
CORPORATE SOURCE: Dep. Chem., Univ. Roorkee, Roorkee, India
SOURCE: J. Protein Chem. (1984), 3(4), 395-401
CODEN: JPCHD2; ISSN: 0277-8033
DOCUMENT TYPE: Journal
LANGUAGE: English
AB N-terminal sequence anal. of arachin, a peanut protein, using a modified Edman method yielded the sequence of the 1st 60 residues. The phenylthiohydantoin (PTH)-amino acids were identified on the basis of m.p., TLC, and UV spectra. For this purpose std. PTH-amino acids were prepd. In addn., 2 new solvent systems for TLC of PTH-amino acids are reported.
IT **4333-21-5**
RL: ANT (Analyte); ANST (Analytical study)
(thin-layer chromatog. of, solvent systems for)
RN 4333-21-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo- (9CI) (CA INDEX NAME)



L12 ANSWER 134 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1985:109135 CAPLUS
DOCUMENT NUMBER: 102:109135
TITLE: Examination of theoretical principles of gradient elution as applied to reversed-phase high-performance liquid chromatography separation of phenylthiohydantoin amino acids
AUTHOR(S): Cohen, K. A.; Dolan, J. W.; Grillo, S. A.
CORPORATE SOURCE: IBM Instrum., Danbury, CT, 06810, USA
SOURCE: J. Chromatogr. (1984), 316, 359-72
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB More than 20 different phenylthiohydantoin (PTH)-derivatized amino acids were used in the examn. of the relevance and the applicability of theor. principles that have been postulated earlier to describe gradient elution in HPLC. Reversed-phase HPLC conditions representative of PTH-amino acid assays, i.e., chem. modified silica microspheres in conjunction with an aq.-org. mobile phase, were utilized. As predicted by theory, inevitable compromises between resoln. and retention time were obsd. empirically. However, an a priori assumption of equiv. linear solvent strength conditions was shown to be inappropriate for selected PTH-amino acid solutes. These findings were supported by the exptl. detd. variability among the different solutes of solvent strength values S, i.e., the slope of the plots of the logarithm of isocratic capacity factor vs. the fraction of org. modifier.
IT **29635-99-2**
RL: ANT (Analyte); ANST (Analytical study)
(sepn. of, by reversed-phase HPLC, gradient elution in)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

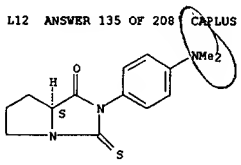
Absolute stereochemistry.



L12 ANSWER 135 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1985:92308 CAPLUS
DOCUMENT NUMBER: 102:92308
TITLE: p-N,N-Dimethylaminophenylisothiocyanate as an electrochemical label for high-performance liquid chromatographic determination of amino acids
AUTHOR(S): Mahachi, Tendai J.; Carlson, Robert M.; Poe, Donald P.
CORPORATE SOURCE: Dep. Chem., Univ. Minnesota, Duluth, MN, 55812, USA
SOURCE: J. Chromatogr. (1984), 298(2), 279-88
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Three arom. isothiocyanates were surveyed as possible precolumn derivatizing agents for the electrochem. detection of amines and amino acids. p-N,N-Dimethylaminophenylisothiocyanate (DMAPI) was chosen for further development as a label in the HPLC detn. of amino acids. Amino acids reacted with DMAPI to form the corresponding substituted phenylthiohydantoins, which were isolated and characterized, and which can be reversibly oxidized at a glassy C electrode at pH 2 with E1/2 = 0.68 V vs. Ag/AgCl. The derivatized amino acids were sepd. on a bonded C8 column in 0.1M phosphate buffer-25% MeCN (pH 2 or 6) and detected at a glassy C electrode set at 0.85 V vs. Ag/AgCl. A mixt. of 21 amino acids was sepd. with 80-98% recovery and with a linear response from 1 to >150 ng and detection limits of 0.5-1 ng.
IT **93413-34-4P**
RL: PREP (Preparation)
(prepn. of)
RN 93413-34-4 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-[4-(dimethylamino)phenyl]hexahydro-3-thioxo-, (S)- (9CI) (CA INDEX NAME)

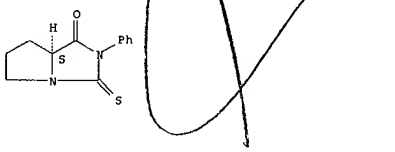
Absolute stereochemistry.

L12 ANSWER 135 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



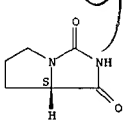
L12 ANSWER 136 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1984:587204 CAPLUS
DOCUMENT NUMBER: 101:187204
TITLE: Separation of phenylthiohydantoin-amino acids by overpressured-layer chromatography
AUTHOR(S): Fater, S.; Mincsovics, E.
CORPORATE SOURCE: Labor Instrument Works, Budapest, H-1445, Hung.
SOURCE: J. Chromatogr. (1984), 298(3), 534-8
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Phenylthiohydantoin (PTH)-amino acids were sepd. by overpressured-layer chromatog. (OPLC) on HPTLC silica gel F254. Two solvent systems were used: CHCl3-95% EtOH-HOAc (90:10:2) and CH2Cl2-EtOAc (90:10). Detection was by densitometry at 275 nm, and the detection limit was 0.05 .mu.g for every PTH-amino acid. Results indicated that linear OPLC with rechromatog. is suitable for the efficient sepn. and quantitation of PTH-amino acids in the structural investigation of proteins and peptides.
IT **29635-99-2**
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, by overpressured-layer chromatog.)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 137 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1984:571695 CAPLUS
DOCUMENT NUMBER: 101:171695
TITLE: Some novel side reactions in peptide chemistry
AUTHOR(S): Kisfaludy, Lajos; Schon, Istvan; Low, Miklos; Szirtes, Tamas; Nyeki, Olga
CORPORATE SOURCE: Chem. Works, Gedeon Richter Ltd., Budapest, Hung.
SOURCE: Pept. Chem. (1984), Volume Date 1983, 21st., 325-32
CODEN: PECHDP
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Newly discovered side reactions in peptide chem. are discussed. Several examples of side reactions in Na/liq. NH3 redn. are shown, e.g. the redn. of Z-Pro-NH2 (Z = PhCH2O2C) by Na/liq. NH3 gave 10% proline hydantoin in addn. to H-Pro-NH2. The optimal amt. of Na in liq. NH3 depends on the character of the peptide, and it is not necessary to conduct the reaction until the blue end point has been reached. In the coupling of Z-Glu(OCMe3)-His-N3 (I) with H-Phe-Arg-Trp-Gly-Lys(Boc)-Pro-Val-Gly-OH (Boc = CO2CMe3) to give protected ACTH 5-14 [Z-Glu(OCMe3)-His-Phe-Arg-Trp-Gly-Lys(Boc)-Pro-Val-Gly-OH], Z-Glu(OCMe3)-His-OH was formed as a side product from the hydrolysis of I. The hydrolysis of histidine-contg. peptide azides does not influence the acylation reaction. The O-alkylation of tyrosine derivs. contg. a free carboxyl group can be effected without racemization in acceptable yields only in NaOH soln. at room temp. The methanolysis of Z-pyroGlu-Phe-Pro-NH2 for 7 days at room temp. gave 84% Z-Glu(OMe)-Phe-Pro-NH2 and 14% pyroGlu-Phe-Pro-NH2.
IT **40856-87-9P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, as side product in sodium-liq. ammonia redn. of proline deriv.)
RN 40856-87-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 137 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

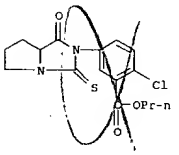
L12 ANSWER 138 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1984:510916 CAPLUS
DOCUMENT NUMBER: 101:110916
TITLE: Herbicidal o-Halobenzoic acid derivatives.
INVENTOR(S): Shimano, Shizuo; Kobayashi, Shinichi; Yanagi, Mikio; Yamada, Osamu; Saito, Mikio; Futatsuya, Fumio
PATENT ASSIGNEE(S): Nippon Kayaku Co., Ltd. , Japan
SOURCE: Eur. Pat. Appl., 46 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 104532	A1	19840404	EP 1983-108992	19830912
EP 104532	B1	19861203		
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
JP 59048481	A2	19840319	JP 1982-158228	19820913
JP 59065070	A2	19840413	JP 1982-175175	19821005
ZA 8306359	A	19840425	ZA 1983-6359	19830826
AU 8318506	A1	19840322	AU 1983-18506	19830829
AU 563282	B2	19870702		
US 4531964	A	19850730	US 1983-527493	19830829
IL 69615	A1	19860831	IL 1983-69615	19830831
CA 1210766	A1	19860902	CA 1983-436085	19830906
DK 8304072	A	19840314	DK 1983-4072	19830908
BR 8304926	A	19840424	BR 1983-4926	19830912
HU 31927	O	19840628	HU 1983-3173	19830912
HU 192160	B	19870528		
AT 24004	E	19861215	AT 1983-108992	19830912

PRIORITY APPLN. INFO.: JP 1982-158228 19820913
JP 1982-175175 19821005
EP 1983-108992 19830912

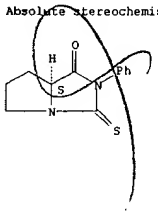
GI For diagram(s), see printed CA Issue.
AB The title compds. I (R1 = H, halo, R2 = halo, R3 = H, C1-8 alkyl, alkoxyalkyl; X = O, S; Q = Q1, Q2; n = 3, 4), useful as pre- and postemergent herbicides, were prepd. Thus, isocyanate II was added to Et 2-piperidinecarboxylate in C6H6 1 h at 40-50.degree. to give 83.2% III which underwent intramol. cyclocondensation to give 71.9% hydantoin I [R1 = F, R2 = Cl, R3 = Me2CH, Q = Q1 (X = O, n = 4) which, based on herbicidal data is the most preferred compd.
IT **91623-92-6P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and herbicidal activity of)

L12 ANSWER 138 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
RN 91623-92-6 CAPLUS
CN Benzoic acid, 2-chloro-5-(tetrahydro-1-oxo-3-thioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)-, propyl ester (9CI) (CA INDEX NAME)



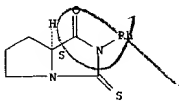
L12 ANSWER 139 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1984:202802 CAPLUS
DOCUMENT NUMBER: 100:202802
TITLE: Isocratic separation of PTH-amino acids by micro high-performance liquid chromatography
AUTHOR(S): Takeuchi, T.; Yamazaki, M.; Ishii, D.
CORPORATE SOURCE: Fac. Eng., Nagoya Univ., Nagoya, 464, Japan
SOURCE: HRC CC, J. High Resolut. Chromatogr. Chromatogr. Commun. (1984), 7(2), 101-2
CODEN: HCJCDB; ISSN: 0344-7138
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Twenty one phenylthiohydantoin (PTH) amino acids were sepd. by high-performance liq. chromatog. on a fused silica microcolumn packed with Silica ODS SC-01 by using isocratic elution with MeCN-THF-5mM NaOAc (pH 5.15). Detection was by UV at 254 nm.
IT **29635-99-2**
RL: ANST (Analytical study); PROC (Process)
(sepn. of, by high-performance liq. chromatog. with isocratic elution)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



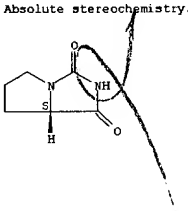
L12 ANSWER 140 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1984:31688 CAPLUS
DOCUMENT NUMBER: 100:31688
TITLE: Separation of phenylthiohydantoin-amino acids by high-performance liquid chromatography
AUTHOR(S): Pucci, Pietro; Sannia, Giovanni; Marino, Gennaro
CORPORATE SOURCE: Ist. Chim. Org. Biol., Univ. Napoli, Naples, I-80134, Italy
SOURCE: J. Chromatogr. (1983), 270, 371-7
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Phenylthiohydantoin-amino acids were sepd. by HPLC on an Ultrasphere ODS (5 .mu.m, 4.6 .times. 250 mm) column; UV detection was at 254 nm. Gradient elution with NaOAc buffer (pH 4.85) and MeCN was at 1.5 mL/min at 35.degree.. The practical application of this method is shown by the sequence anal. of bovine pancreatic RNase. Peaks of phenylthiohydantoin-amino acids were well sepd. from background peaks, and a high signal/noise ratio was achieved in the chromatogram of 10% of the sample at the 20th cycle of a 15-nmol anal.
IT **29635-99-2**
RL: ANT (Analyte); ANST (Analytical study)
(chromatog. of, reversed-phase high-performance liq.)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 141 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1983:558837 CAPLUS
DOCUMENT NUMBER: 99:158837
TITLE: Reexamination of sodium-liquid ammonia reduction in peptide chemistry
AUTHOR(S): Schon, Istvan; Szirtes, Tamas; Uberhardt, Tamas; Rill, Attila; Csehi, Attila; Hegedus, Bela
CORPORATE SOURCE: Chem. Works, Gedeon Richter Ltd., Budapest, Hung.
SOURCE: Int. J. Pept. Protein Res. (1983), 22(1), 92-109
CODEN: IJPPC3; ISSN: 0367-8377
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Sodium-liq. ammonia redn. has been used for over 50 yr for removal of benzyl-type protecting groups in peptide chem. Up until now a definite blue end-point has generally been accepted for detection of the completion of reaction. Systematic investigation with model compds. has revealed that this is not only unnecessary for the complete removal of the protecting groups but also that the application of sodium in excess results in many undesired transformations which can simply be suppressed or even eliminated by optimizing the sodium consumption. Cleavage of the tert-butyloxycarbonyl group and the N-C.alpha. bond, redn. of carboxamide groups to carbinol derivs., transpeptidation, and formation of a hydantoin deriv. was obsd. in model expts. by using sodium in excess.
IT **40856-87-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 40856-87-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-, (7aS)- (9CI) (CA INDEX NAME)

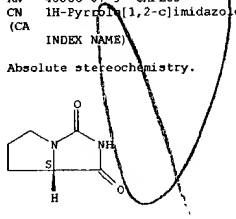
Absolute stereochemistry.



L12 ANSWER 141 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

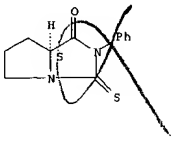
L12 ANSWER 142 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1983:522849 CAPLUS
DOCUMENT NUMBER: 99:122849
TITLE: Solution conformation and dynamics of L-6-methylperhydroimidazo[1,5-c]thiazole-5,7-dione (.gamma.-thiaprolinehydantoin). A proton and carbon-13 NMR study
AUTHOR(S): Borremans, Frans A. M.; Budesinsky, Milos; Callens, Roland E. A.; Anteunis, Marc J. O.
CORPORATE SOURCE: Dep. Org. Chem., Rijksuniv. Gent, Ghent, B-9000, Belg.
SOURCE: Org. Magn. Reson. (1983), 21(5), 328-33
CODEN: ORMRBD; ISSN: 0030-4921
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The soln. conformation of the title compd. is detd. from the 1H and 13C NMR, allowing the extn. of vicinal inter-proton and 13C-1H coupling consts. The major conformation of the thiazolidine ring is an envelope with C-.delta. as the flap exo (.delta.-). In soln. the preferred solid state (twist) conformer with C-.alpha. exo and C-.beta. endo (.alpha..beta.T) is only a minor contributor. 13C spin-lattice relaxation data reveal the flexibility of the thiazolidine ring and the pseudorotation of this ring is discussed.
IT **40856-87-9**
RL: RCT (Reactant)
(nuclear Overhauser effect and magnetic relaxation of carbon-13 in)
RN 40856-87-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

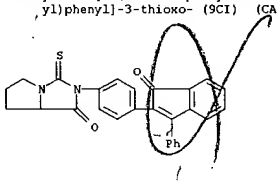


L12 ANSWER 143 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1983:449835 CAPLUS
DOCUMENT NUMBER: 99:49835
TITLE: Chemical ionization mass spectral analysis of phenylthiohydantoin derivatives
AUTHOR(S): Fairwell, Thomas
CORPORATE SOURCE: Dep. Health Hum. Serv., Natl. Heart, Lung, Blood Inst., Bethesda, MD, 20205, USA
SOURCE: Methods Enzymol. (1983), 91(Enzyme Struct., Pt. I), 502-11
CODEN: MENZAU; ISSN: 0076-6879
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Chem.-ionization mass-spectroscopic identification of amino acid phenylthiohydantoins and interpretation of the spectra are discussed.
IT **29635-99-2**
RL: PRP (Properties)
(mass spectrum of, chem.-ionization)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

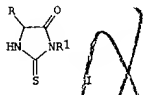
Absolute stereochemistry.



L12 ANSWER 144 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1983:447326 CAPLUS
DOCUMENT NUMBER: 99:47326
TITLE: On the regeneration of amino acids from their diphenylindonyl-substituted thiohydantoin derivatives
AUTHOR(S): Mancheva, I. N.; Simeonova, R. A.
CORPORATE SOURCE: Dep. Org. Chem., Higher Inst. Chem. Technol., Sofia, 1156, Bulg.
SOURCE: Dokl. Bolg. Akad. Nauk (1982), 35(12), 1685-8
CODEN: DBANAD; ISSN: 0366-8681
DOCUMENT TYPE: Journal
LANGUAGE: English
AB An indirect method for detg. amino acids which were derivatized as diphenylindonylthiohydantoin for high-performance liq. chromatog. is based on acid or alk. hydrolysis of the amino acid derivs. Optimum conditions for hydrolysis were established. The amino acids were then detd. by using an automatic amino acid analyzer.
IT **42353-03-7**
RL: ANST (Analytical study)
(amino acid generation from, by hydrolysis, for anal.)
RN 42353-03-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-[4-(1-oxo-3-phenyl-1H-inden-2-yl)phenyl]-3-thioxo- (9CI) (CA INDEX NAME)

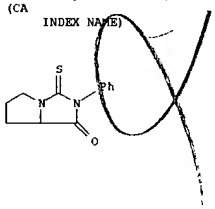


L12 ANSWER 145 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1983:438799 CAPLUS
DOCUMENT NUMBER: 99:38799
TITLE: Reactivity of dithiocarbamic esters: methods for the preparation of 3,5-substituted 2-thiohydantoins
AUTHOR(S): Blotny, Grzegorz
CORPORATE SOURCE: Inst. Inorg. Chem. Technol., Tech. Univ., Gdansk, 80-952, Pol.
SOURCE: Synthesis (1983), (5), 391-2
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Thiohydantoins I (R = H, R1 = CHMe2, Ph; R = CH2CHMe2, R1 = CHMe2, n-C6H13; R = Me, CH2Ph, R1 = CHMe2, CMe3, n-C6H13, Ph) were prepd. in 78-97% yields by treating H2NCHRCO2H (II) with R1NHCS2Me (III), by treating II with CS2 and H2NR1, or by treating an ester of II with III. I (R = Me, R1 = Ph) was also prepd. by cyclizing EtS2C-DL-Ala-OH with H2NPh in refluxing EtOH contg. Et3N for 5 h.
IT **31364-82-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 31364-82-6 CAPLUS

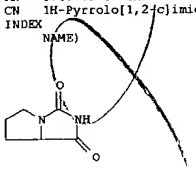
L12 ANSWER 146 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1983:422893 CAPLUS
DOCUMENT NUMBER: 99:22893
TITLE: A study of the Edman degradation in the assessment of the purity of synthetic peptides
AUTHOR(S): Kent, Stephen B. H.; Riemen, Mark; LeDoux, Marie; Merrifield, R. B.
CORPORATE SOURCE: Rockfeller Univ., New York, NY, 10021, USA
SOURCE: Methods Protein Sequence Anal., [Proc. Int. Conf.], 4th (1982), Meeting Date 1981, 205-13. Editor(s): Elzinga, Marshall. Humana: Clifton, N. J.
CODEN: 49KBAY
DOCUMENT TYPE: Conference
LANGUAGE: English
AB The Edman degrdn. was applied to the total sequence anal. of long peptides prepd. by the solid-phase method in order to evaluate whether the reported min. level of preview in the anal. of omission in solid-phase peptide synthesis by Edman degrdn. was a real measure of synthetic efficiency or an artifact of the Edman degrdn.
IT **4333-21-5**
RL: PROC (Process)
(sepn. of, by reverse-phase high-performance liq. chromatog.)
RN 4333-21-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo- (9CI) (CA INDEX NAME)



L12 ANSWER 147 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1982:598566 CAPLUS
DOCUMENT NUMBER: 97:198566
TITLE: Aqueous sodium .alpha.-amino carboxylate solutions
INVENTOR(S): Kleemann, Axel; Lehmann, Bernd; Martens, Juergen
PATENT ASSIGNEE(S): Degussa A.-G., Fed. Rep. Ger.
SOURCE: Ger. Offen., 11 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3105008	A1	19820819	DE 1981-3105008	19810212
DE 3105008	C2	19910411		
FR 2499560	A1	19820813	FR 1982-2002	19820208
FR 2499560	B1	19850419		
US 4436910	A	19840313	US 1982-347477	19820210
JP 57150645	A2	19820917	JP 1982-19875	19820212
JP 02019820	B4	19900507		

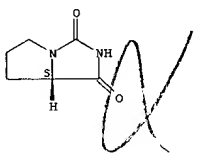
PRIORITY APPLN. INFO.: DE 1981-3105008 19810212
AB Title solns. were prepd. by the alk. hydrolysis of the corresponding hydantoins at 110-80.degree.. Thus, hydantoin was treated with Ca(OH)2 and NaOH in H2O in an autoclave at 140.degree. for 4 h and the resulting soln. was cooled to 50.degree. and then filtered. The CaCO3 residue was washed with H2O and the above filtrate and aq. wash were combined to give an aq. soln. of glycine Na salt (97% yield).
IT **5768-79-6**
RL: RCT (Reactant)
(hydrolysis of)
RN 5768-79-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro- (9CI) (CA INDEX NAME)



L12 ANSWER 147 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

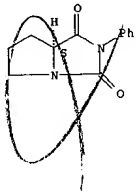
L12 ANSWER 148 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1982:563460 CAPLUS
DOCUMENT NUMBER: 97:163460
TITLE: Formation of by-products during sodium-liquid ammonia reduction in peptide chemistry
AUTHOR(S): Schon, Istvan; Szirtes, Tamas; Uberhardt, Tamas
CORPORATE SOURCE: Chem. Works, Gedeon Richter, Ltd., Budapest, H-1475, Hung.
SOURCE: J. Chem. Soc., Chem. Commun. (1982), (11), 639-40
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Redn. of peptides and amino acids by excess Na in NH3(l) to remove benzyl-type and tosyl protecting groups gave undesired by-products. These side reactions can be minimized or eliminated by using only slightly more Na than the theor. amt.
IT **40856-87-9P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in deprotection of amino acid by sodium in liq. ammonia)
RN 40856-87-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

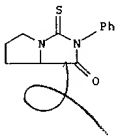


L12 ANSWER 149 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1982:424199 CAPLUS
DOCUMENT NUMBER: 97:24199
TITLE: Solid-phase Edman degradation as an aid in evaluation of the homogeneity of peptidyl-resin intermediates obtained from Merrifield solid-phase synthesis
AUTHOR(S): Margolies, Michael N.; Matsueda, Gary R.
CORPORATE SOURCE: Dep. Surg., Massachusetts Gen. Hosp., Boston, MA, 02114, USA
SOURCE: Dev. Biochem. (1981), (Chem. Synth. Sequencing Pept. Proteins), 207-19
CODEN: DEBIDR; ISSN: 0165-1714
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The title study was discussed in terms of an anal. of a peptidyl resin in which the repetitive yield during degrdn. would be high and an anal. of a method to quantitate all of the amino acid phenylthiohydantoins encountered in the degrdn. of peptidyl resins.
IT **70741-88-7**
RL: ANT (Analyte); ANST (Analytical study)
(anal. of, in solid-phase Edman degrdn. of peptidyl resin)
RN 70741-88-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-phenyl-, (7aS)- (9CI) (CA INDEX NAME)

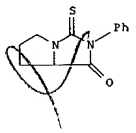
Absolute stereochemistry.



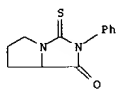
L12 ANSWER 150 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1982:200123 CAPLUS
DOCUMENT NUMBER: 96:200123
TITLE: Rapid analysis of amino-acid phenylthiohydantoins by high performance liquid chromatography: stepwise elution with a 15-cm column
AUTHOR(S): Bledsoe, Marianna; Pisano, John J.
CORPORATE SOURCE: Lab. Chem., Natl. Heart, Lung, Blood Inst., Bethesda, MD, 20205, USA
SOURCE: Dev. Biochem. (1981), (Chem. Synth. Sequencing Pept. Proteins), 245-9
CODEN: DEBIDR; ISSN: 0165-1714
DOCUMENT TYPE: Journal
LANGUAGE: English
AB All 20 amino acid phenylthiohydantoins were identified by high-performance liq. chromatog. in a single 12 min run using a 15 cm Zorbax ODS column and stepwise elution.
IT **4333-21-5**
RL: ANT (Analyte); ANST (Analytical study)
(high-performance liq. chromatog. of)
RN 4333-21-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo- (9CI) (CA INDEX NAME)

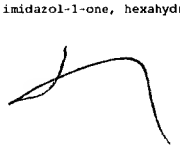


L12 ANSWER 151 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1982:200120 CAPLUS
DOCUMENT NUMBER: 96:200120
TITLE: Separation of phenylthiohydantoin-amino acid by high-pressure liquid chromatography
AUTHOR(S): Chen, Xiangfang; Chen, Shen; Zhen, Zhen
CORPORATE SOURCE: Inst. Photochem., Acad. Sin., Peop. Rep. China
SOURCE: Fenxi Huaxue (1981), 9(4), 451-2, 458
CODEN: FHHHDT
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB A mixt. of amino acid phenylthiohydantoins was sepd. efficiently by high-pressure liq. chromatog. using "solvent A" contg. MeOH 100, H2O 900, HOAc 2.5, acetone 50 mL (adjusted to pH 4 with NaOH) and "solvent B" contg. MeOH 900, H2O 100, and HOAc 0.2 mL as the moving phase.
IT **4333-21-5**
RL: PROC (Process)
(sepn. of, by high-pressure liq. chromatog.)
RN 4333-21-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo- (9CI) (CA INDEX NAME)



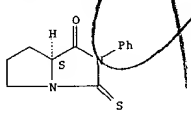
L12 ANSWER 152 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1981:543588 CAPLUS
DOCUMENT NUMBER: 95:143588
TITLE: Use of a ternary gradient for the separation of phenylthiohydantoin-amino acids, including the methyl esters of aspartic and glutamic acids, by high-performance liquid chromatography
AUTHOR(S): DiMari, Samuel J.; Robinson, John P.; Nash, John H.
CORPORATE SOURCE: Sch. Med., Vanderbilt Univ., Nashville, TN, 37232, USA
SOURCE: J. Chromatogr. (1981), 213(1), 91-7
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The phenylthiohydantoin (PTH) derivs. of the common amino acids can be resolved in a single high-performance liq. chromatog. anal. by elution from a cyanopropylsilane column with a ternary gradient of MeOH, MeCN, and NH4OAc. The system is compatible with an automated sequencer-automated converter combination that produces the Me esters of PTH-aspartic and PTH-glutamic acids.
IT **4333-21-5**
RL: ANST (Analytical study); PROC (Process)
(sepn. of, by high-performance liq. chromatog. with ternary gradient system)
RN 4333-21-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo- (9CI) (CA INDEX NAME)





L12 ANSWER 153 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1981:402770 CAPLUS
DOCUMENT NUMBER: 95:2770
TITLE: Identification of the phenylthiohydantoin derivatives of amino acids by high pressure liquid chromatography, using a ternary, isocratic solvent system
AUTHOR(S): Lottspeich, Friedrich
CORPORATE SOURCE: Max-Planck-Inst. Biochem., Martinsried, D-8033, Fed. Rep. Ger.
SOURCE: Hoppe-Seyler's Z. Physiol. Chem. (1980), 361(12), 1829-34
CODEN: HSZPAZ; ISSN: 0018-4888
DOCUMENT TYPE: Journal
LANGUAGE: English
AB By using a ternary solvent system, a rapid isocratic sepn. of the usual amino acid phenylthiohydantoin derivs. was achieved with the exception of the pair glutaminephenylthiohydantoin deriv./serine phenylthiohydantoin deriv. In practice, discriminating between these 2 derivs. is seldom a problem because the glutamine deriv. is partially deamidated during the conversion and is therefore always accompanied by the glutamate deriv. The dependence of the retention times from pH, buffer compn., buffer concn., and temp. are discussed.
IT **29635-99-2**
RL: ANT (Analyte); ANST (Analytical study)
(chromatog. of, high-pressure liq.)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)- (9CI) (CA INDEX NAME)

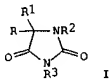
Absolute stereochemistry.



L12 ANSWER 154 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1981:103378 CAPLUS
DOCUMENT NUMBER: 94:103378
TITLE: Treating asthma with alkyl, alkylidene and alkylene hydantoins
INVENTOR(S): Jamieson, William B.; Ross, William J.; Simmonds, Robin G.; Verge, John P.
PATENT ASSIGNEE(S): Lilly Industries Ltd., Engl.
SOURCE: U.S., 6 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4230709	A	19801028	US 1979-39074	19790514
GB 1600880	A	19811021	GB 1978-21353	19780523
PRIORITY APPLN. INFO.:			GB 1978-21353	19780523

GI



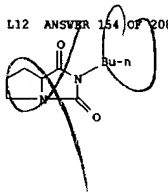
I

AB Title compds. I (R = Me and R1 = H or Me, or RR1 = alkylidene or alkylene; R2 = H or alkyl, or RR2 = alkylene; R3 = alkyl, PhCH2), were prepd. by different methods and they are useful in the treatment of asthma (no data). I (R = Me, R1 = R2 = H, R3 = Bu) reacted with NaH and BuBr to give I R = Me, R1 = H, R2 = R3 = Bu). .alpha.-Aminoisobutyric acid was treated with BuNCO and NaOH to yield I (R = R1 = Me, R2 = H, R3 = Bu).

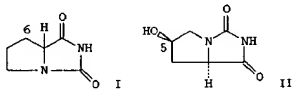
IT **76670-00-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 76670-00-3 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-butyltetrahydro- (9CI) (CA INDEX NAME)

L12 ANSWER 154 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



L12 ANSWER 155 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1980:585641 CAPLUS
DOCUMENT NUMBER: 93:185641
TITLE: Structure of two prolinehydantoin derivatives: L-prolinehydantoin C6H8N2O2 and D-allohydroxyprolinehydantoin
AUTHOR(S): Arte, E.; Tinant, B.; Declercq, J. P.; Germain, G.; Van Meerssche, M.
CORPORATE SOURCE: Lab. Chim. Phys. Cristallogr., Univ. Louvain, Louvain-la-Neuve, B-1348, Belg.
SOURCE: Bull. Soc. Chim. Belg. (1980), 89(5), 379-84
CODEN: BSCBAG; ISSN: 0037-9646
DOCUMENT TYPE: Journal
LANGUAGE: French
GI



I II

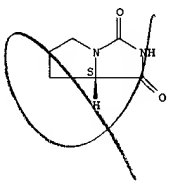
AB The structure of L-proline hydantoin (I) and D-allohydroxyproline hydantoin (II) as examd. crystallog. The conformation of proline ring has the C-6 atom out of the ring plane of the other 4 atoms and endo to the flattened hydantoin half-chain in I; a similar conformation exists for II with C-5 out of the ring plane and endo to the flattened hydantoin ring half-chain.

IT **40856-87-9**
RL: PRP (Properties)
(crystal and mol. structure of, conformation in relation to)

RN 40856-87-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 155 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

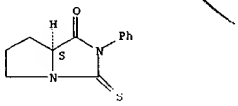


L12 ANSWER 156 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1980:491531 CAPLUS
DOCUMENT NUMBER: 93:91531
TITLE: Fluorometric determination of phenylthiohydantoin amino acids
INVENTOR(S): Kinoshita, Toshio; Murayama, Kazuyo
PATENT ASSIGNEE(S): Yuki Gosei Kogyo Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

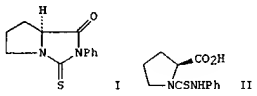
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 55036740	A2	19800314	JP 1978-109602	19780908

AB Phenylthiohydantoin-amino acids in hydrolyzates of peptides or proteins after Edman hydrolysis are detd. by treatment with pyridoxamine and Pb(OAc)2, and the reaction mixt. is analyzed fluorometrically for the measurement of phenylthiohydantoin-amino acids. Thus, phenylthiohydantoin-norleucine in EtOAc was treated with pyridoxamine and Pb(OAc)2 in 2% pyridine-MeOH at 70.degree. for 90 min. After cooling, the mixt. was analyzed at 465 nm with excitation at 390 nm.
IT **29635-99-2**
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, fluorometric)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



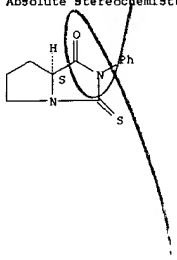
L12 ANSWER 157 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1980:76398 CAPLUS
DOCUMENT NUMBER: 92:76398
TITLE: A new synthesis of (S) - (+) -1,5-cyclotrimethylene-3-phenyl-2-thiohydantoin
AUTHOR(S): Poupaert, Jacques H.; Lhoest, Georges
CORPORATE SOURCE: Sch. Pharm., Univ. Louvain, Brussels, B-1200, Belg.
SOURCE: Bull. Soc. Chim. Belg. (1979), 88(5), 339-42
CODEN: BSCBAG; ISSN: 0037-9646
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I II

AB The title compd. (I) was obtained in 39% overall yield by treating proline with PhNCS and thermally cyclizing the phenylthiohydantoic acid II. (R)-(+)-5-Cyclohexyl-3-phenyl-2-thiohydantoin was similarly prepd. in 54% yield from (R)-(-)-cyclohexylglycine.
IT **29635-99-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

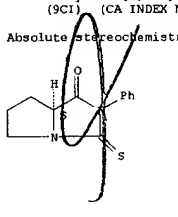
Absolute stereochemistry.



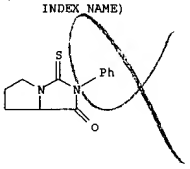
L12 ANSWER 157 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

L12 ANSWER 158 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1980:2596 CAPLUS
DOCUMENT NUMBER: 92:2596
TITLE: Identification of amino acid phenylthiohydantoins by gradient, high-performance liquid chromatography on Spherisorb S5-ODS
AUTHOR(S): Moser, Peter W.; Rickli, Egon E.
CORPORATE SOURCE: Inst. Biochem., Univ. Berne, Bern, CH-3012, Switz.
SOURCE: J. Chromatogr. (1979), 176(3), 451-5
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Amino acid phenylthiohydantoin (PTH) derivs. were sepd. by high-performance liq. chromatog. in a single anal. A stainless steel column packed with Spherisorb S5-ODS and an eluting solvent of MeCN in LiOAc buffer were used. The differences in retention times of PTH-valine and -methionine and of PTH-isoleucine, -tryptophan, -phenylalanine, and -leucine were .apprx.0.2 min, sufficient for unequivocal resoln. of these derivs. that are difficult to sep. The method was reproducible after .apprx.1000 runs, and the time required (23 min) keeps pace with the rhythm of automated Edman degrdn.
IT **29635-99-2**
RL: ANT (Analyte); ANST (Analytical study)
(chromatog. of, on Spherisorb S5-ODS)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

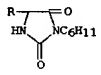
Absolute stereochemistry.



L12 ANSWER 159 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1979:204450 CAPLUS
DOCUMENT NUMBER: 90:204450
TITLE: Back hydrolysis of amino acid phenylthiohydantoins by the use of 6N hydrochloric acid containing mercaptoethanol and phenol
AUTHOR(S): Lu, Hsieng-Sen; Sun, Wan-Mei; Chen, Shun-Wen; Lo, Tung-Bin
CORPORATE SOURCE: Inst. Biochem. Sci., Natl. Taiwan Univ., Taipei, Taiwan
SOURCE: Proc. Natl. Sci. Counc., Repub. China (1978), 2(4), 352-5
CODEN: PSIADU
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The use of 6N HCl contg. 1% HSCH2CH2OH and 0.2% PhOH gave the best results for the title hydrolysis. The recovery of S-carboxymethylcysteine from the title cysteine deriv. was >80%; consequently, this method is useful in the sequencing of proteins with high cystine content. This method was applied to the sequencing of 2 tryptic peptides from cardiotoxin.
IT **4333-21-5**
RL: RCT (Reactant)
(back hydrolysis of)
RN 4333-21-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo- (9CI) (CA INDEX NAME)

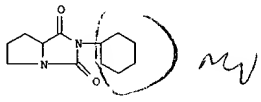


L12 ANSWER 160 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1979:187304 CAPLUS
DOCUMENT NUMBER: 90:187304
TITLE: Side reactions during the removal of protecting groups of N-(protected aminoacyl)urea derivatives
AUTHOR(S): Schon, I.; Friss, J.; Kisfaludy, L.
CORPORATE SOURCE: Chem. Works, Gedeon Richter Ltd., Budapest, Hung.
SOURCE: Acta Chim. Acad. Sci. Hung. (1978), 98(2), 215-23
CODEN: ACASA2; ISSN: 0001-5407
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



II

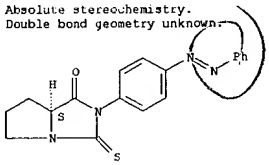
AB PhCH2O2CNHCHRCON(C6H11)CONHC6H11 (I, R = H, Me, CHMe2, CH2CHMe2, CHMeEt, CH2Ph, CH2OH, CHMeOH, Ph; C6H11 = cyclohexyl) were completely hydrogenated over Pd-C to give 64.6-91.5% conversion to hydantoins II and 8.5-35.4% conversion to C6H11NHCONHCHRCONHC6H11. Acidolysis of I (R = H) with HBr gave 83.2% H-Gly-NHC6H11.HBr, whereas with HCl 72.3% PhCH2O2C-Gly-NHC6H11 was obtained.
IT **70118-26-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, in hydrogenation of benzyloxycarbonyl amino acid dicyclohexylurea deriv.)
RN 70118-26-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, 2-cyclohexyltetrahydro- (9CI) (CA INDEX NAME)



L12 ANSWER 160 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

L12 ANSWER 161 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1979:182514 CAPLUS
DOCUMENT NUMBER: 90:182514
TITLE: Spray reagents for the detection of p-phenylazophenylthiohydantoins of amino acids on silica gel plates
AUTHOR(S): Datta, Shompa; Datta, Salil C.
CORPORATE SOURCE: Dep. Chem., Univ. Kalyani, Kalyani, India
SOURCE: J. Chromatogr. (1979), 170(1), 228-32
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Spray reagent systems for the detection of p-phenylazophenylthiohydantoins of amino acids on thin-layer chromatog. plates are compared. The spray reagent systems contained as color reagents phenylnaphthylamine, or ninhydrin .+-.Cu(NO3)2, or cyclohexylamine, or isatin and Zn(OAc)2. The colors of the amino acid derivs. following spraying are described for each spray reagent system.
IT **70172-70-2**
RL: ANT (Analyte); ANST (Analytical study)
(thin-layer chromatog. of, spray reagents for)
RN 70172-70-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-[4-(phenylazo)phenyl]-3-thioxo-, (S)- (9CI) (CA INDEX NAME)

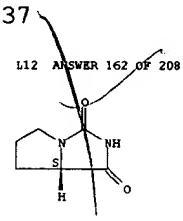
Absolute stereochemistry.
Double bond geometry unknown.



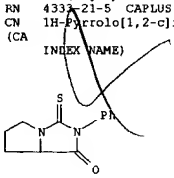
L12 ANSWER 162 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1979:104334 CAPLUS
DOCUMENT NUMBER: 90:104334
TITLE: Ring conformational aspects of proline and hydroxyproline. High conformational purity of proline in diketopiperazined and hydantoins
AUTHOR(S): Anteunis, Marc J. O.; Callens, Roland; Asher, Vikram; Sleeckx, Jozef
CORPORATE SOURCE: Lab. Org. Chem., Rijksuniv.-Gent, Ghent, Belg.
SOURCE: Bull. Soc. Chim. Belg. (1978), 87(1), 41-60
CODEN: BSCBAG; ISSN: 0037-9646
DOCUMENT TYPE: Journal
LANGUAGE: English
AB NMR data for proline (I) and trans-hydroxyproline (II) linear and cyclic peptides were analyzed. In acyclic and cyclic derivs. the pyrrolidine ring of II possesses a homogenous conformation which changes when .PHI. values become for L-residues more neg. than -40.degree.. The pyrrolidine ring in I possesses more flexibility esp. in acyclic derivs., and in cyclic derivs. its higher mobility prevails compared to that in II. The nature of the major populations in the pseudorotational path of 5-membered rings is more sensitive in I towards changes in .PHI.. The conformation of these derivs. depends only markedly on .PHI. for low values (.PHI. < -45.degree.). With more pos. .PHI. values, the ring conformations remain remarkably eqwual and close to a gE-form.
IT **40856-87-9**
RL: PRP (Properties)
(proline ring conformation of, NMR in relation to)
RN 40856-87-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 162 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

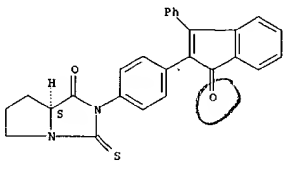


L12 ANSWER 163 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1979:50760 CAPLUS
DOCUMENT NUMBER: 90:50760
TITLE: Separation of phenylthiohydantoin (PTH) amino acids by high pressure liquid chromatography
AUTHOR(S): Oestvold, Geir; Jensen, Einar; Greibrokk, Tyge
CORPORATE SOURCE: Dep. Chem., Univ. Oslo, Oslo, Norway
SOURCE: Medd. Nor. Farm. Selsk. (1978), 40(3), 173-9
CODEN: MNFSAW; ISSN: 0369-1020
DOCUMENT TYPE: Journal
LANGUAGE: English
AB HPLC-sepn. and identification of 24 PTH amino acids were obtained by gradient elution on octadecylsilyl (ODS)-packings. The majority of the partially resolved components also could be identified by isocratic elution. ODS-packings of different manuf. were examd., and considerable differences were obtained, esp. on the retention of basic components. Problems of reproducibility were examd. and discussed.
IT **4333-21-5**
RL: PROC (Process)
(high-pressure liq. chromatog. of)
RN 4333-21-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo- (9CI) (CA INDEX NAME)

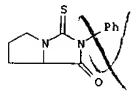


L12 ANSWER 164 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1978:580316 CAPLUS
DOCUMENT NUMBER: 89:180316
TITLE: Separation of two types of diphenylindenone derivatives of amino acids (ITH- and DIS-amino acids) applicable to sequencing of proteins on polyamide sheets
AUTHOR(S): Mancheva, I.; Vladovska-Yukhnovska, Y.
CORPORATE SOURCE: Dep. Org. Chem., Higher Inst. Chem. Technol., Sofia, Bulg.
SOURCE: J. Chromatogr. (1978), 151(2), 207-14
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Suitable solvent systems were detd. for the sepn. of protein amino acids as their diphenylindenonylthiohydantoin (ITH) derivs. or their diphenylindenonesulfonyl (DIS) derivs. at picomole levels by 2-dimensional thin-layer chromatog. on polyamide sheets. The ITH derivs. and the DIS amino acids were prepd. by treating the amino acid with 2-p-isothiocyanatophenyl-3-phenylindenone and DIS-Cl, resp.
IT **67737-97-7**
RL: ANT (Analyte); ANST (Analytical study)
(thin-layer chromatog. of)
RN 67737-97-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-[4-(1-oxo-3-phenyl-1H-inden-2-yl)phenyl]-3-thioxo-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

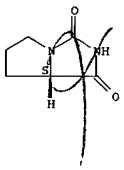


L12 ANSWER 165 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1978:529906 CAPLUS
DOCUMENT NUMBER: 89:129906
TITLE: Separation of PTH-amino acids by isocratic high-performance liquid chromatograpy
AUTHOR(S): Abrahamsson, Monika; Groningsson, Kerstin; Castensson, Staffan
CORPORATE SOURCE: Res. Dep., AB KABI, Stockholm, Swed.
SOURCE: J. Chromatogr. (1978), 154(2), 313-17
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Twenty-one phenylthiohydantoin (PTH) amino acids, which are normally encountered in the Edman degrdn. of proteins, were efficiently sepd. by the title chromatog. The optimum temp. for sepn. was 50.degree..
IT **4333-21-5**
RL: PROC (Process)
(isocratic high-performance liq. chromatog. of)
RN 4333-21-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo- (9CI) (CA INDEX NAME)



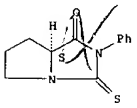
L12 ANSWER 166 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1978:510363 CAPLUS
DOCUMENT NUMBER: 89:110363
TITLE: Hydantoinic scale in peptide conformation investigations by carbon-13 NMR spectroscopy
AUTHOR(S): Siemion, Ignacy Z.; Sobczyk, Katarzyna; Picur, Boleslaw
CORPORATE SOURCE: Inst. Chem., Univ. Wroclaw, Wroclaw, Pol.
SOURCE: Pol. J. Chem. (1978), 52(3), 667-9
CODEN: PJCHDQ
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Since hydantoins can function as stds. with well defined conformational characteristics, the C.beta. chem. shifts in the 13C NMR of the hydantoins of 16 amino acids (e.g., DL-alanine, proline, N6-benzyloxycarbonyl-DL-lysine) were obtained for comparison with the C.beta. signal positions of the amino acid residues in peptides. This hydantoinic scale can be used to compare the conformation of a particular residue in peptide chains directly from 13C NMR data. The conformation of gramicidin S was detd. from this hydantoinic scale.
IT **40856-87-9**
RL: PRP (Properties)
(carbon-13 NMR of, .beta.-carbon chem. shifts in)
RN 40856-87-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



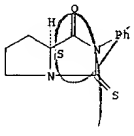
L12 ANSWER 167 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1978:510312 CAPLUS
DOCUMENT NUMBER: 89:110312
TITLE: A simple and rapid method for the identification of 3-phenylthiohydantoins derived from amino acids based on thin layer chromatography
AUTHOR(S): Munier, Roger L.; Drapier, Anne Marie
CORPORATE SOURCE: Inst. Pasteur, CNRS, Paris, Fr.
SOURCE: C. R. Hebd. Seances Acad. Sci., Ser. C (1978), 286(15), 433-6
CODEN: CHDCAQ; ISSN: 0567-6541
DOCUMENT TYPE: Journal
LANGUAGE: French
AB Amino acid phenylthiohydantoins of amino acids are characterized by thin-layer chromatog. on silica gel. Several suitable solvent systems are given.
IT **29635-99-2**
RL: ANT (Analyte); ANST (Analytical study)
(thin layer chromatog. of)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



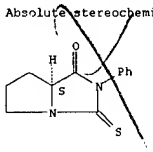
L12 ANSWER 168 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1978:502945 CAPLUS
DOCUMENT NUMBER: 89:102945
TITLE: Direct microsequence analysis of polypeptides using an improved sequenator, a nonprotein carrier (Polybrene), and high pressure liquid chromatography
AUTHOR(S): Hunkapiller, Michael W.; Hood, Leroy E.
CORPORATE SOURCE: Div. Biol., California Inst. Technol., Pasadena, Calif., USA
SOURCE: Biochemistry (1978), 17(11), 2124-33
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Combined use of Polybrene, high-pressure liq. chromatog., and modifications in Edman chem. with improvement of a com. spinning cup sequenator (Wittmann-Liebold, B., 1973) is recommended for analyzing amino acid phenylthiohydantoins obtained from automated Edman degrdn. of microquantities of polypeptide directly without the use of radiolabel. This approach allowed detn. of the sequence of the N-terminal 47 residues of sperm whale myoglobin starting with 200 pmol of protein, 77 residues of an antibody light chain with 5 nmol of protein, and 54 residues of an antibody heavy chain with 8 nmol of protein. In addn., a hydrophobic 14-residue peptide was completeley sequenced at the 1.5-nmol level. This technique of direct anal. for microsamples is capable of providing routine, extended N-terminal sequence anal. for nmol and sub-nmol levels of polypeptides and proteins, and it also is applicable to anal. of more classical sample quantities.
IT **29635-99-2**
RL: ANT (Analyte); ANST (Analytical study)
(chromatog. of, high-performance liq., in peptide microsequencing)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 169 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1978:502932 CAPLUS
DOCUMENT NUMBER: 89:102932
TITLE: Solid phase degradations on macroporous polystyrene derivatives with identification of thiazolinones as PTC amino acid methylamides
AUTHOR(S): Appella, Ettore; Inman, John K.; Dubois, Garrett C.
CORPORATE SOURCE: Natl. Cancer Inst., NIH, Bethesda, Md., USA
SOURCE: INSERM Symp. (1977), 5(Solid Phase Methods Protein Sequence Anal.), 121-33
CODEN: INSSDM
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Derivs. of macroporous polystyrene were used as supports for solid-phase peptide sequencing. Attachment yields for these resins were comparable to those obtained with other known supports. The effect of the type and length of the spacer arm sepg. the resin matrix and the peptide was investigated. 2-Aminoethylthio-polyethylene glycol-methylaminomethyl (AET-PEG-MAM) polystyrene, contg. a long polyether spacer arm, gave exceptionally clean thiazolinones which were converted to phenylthiohydantoins (PTHs) or to phenylthiocarbamyl (PTC) amino acid methylamides. The PTC methylamide derivs. can be easily identified by thin-layer chromatog. or high-pressure liq. chromatog. In addn., PTC methylamide derivs. were more rapidly formed and were more stable than the corresponding PTH derivs. Consequently, the identification of both serine and threonine can be greatly improved.
IT **29635-99-2**
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, by high-pressure liq. chromatog.)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

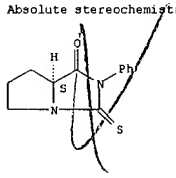
Absolute stereochemistry.



L12 ANSWER 169 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

L12 ANSWER 170 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1978:438885 CAPLUS
DOCUMENT NUMBER: 89:38885
TITLE: Effects of pH, ionic strength, and organic modifier on the chromatographic behavior of amino acids and peptides using a bonded peptide stationary phase
AUTHOR(S): Fong, Godwin W. K.; Grushka, Eli
CORPORATE SOURCE: Dep. Chem., State Univ. New York, Buffalo, N. Y., USA
SOURCE: Anal. Chem. (1978), 50(8), 1154-61
CODEN: ANCHAM; ISSN: 0003-2700
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A bonded tripeptide phase, L-Val-L-Ala-L-Pro, was used as a stationary phase in liq. chromatog. for the sepn. of phenylthiohydantoin (PTH)-amino acids and dipeptides. All 25 PTH-amino acids tested have different capacity ratios when either acidic (pH .simeq.2.5) or basic (pH .simeq.7.4) aq. citrate mobile phases were used as eluents. The chromatog. behavior of some free and protected dipeptides were also studied systematically. The pH of the mobile phase, its ionic strength, and the amt. of org. modifier (MeOH) affect the retention behavior of the dipeptides. The retention characteristics of the free dipeptides were affected to a greater extent than those of the protected ones. The results indicate that mobile phases can be tailor-designed for optimum sepns. of the isomeric dipeptides. Comparisons with previous bonded peptide columns are made in order to gain a better understanding of the mechanism of sepn.
IT **29635-99-2**
RL: ANT (Analyte); ANST (Analytical study)
(chromatog. of, on tripeptide-bonded stationary phase, mobile phase effect on)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

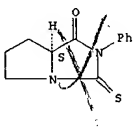
Absolute stereochemistry.



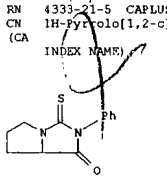
L12 ANSWER 170 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

L12 ANSWER 171 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1978:424767 CAPLUS
DOCUMENT NUMBER: 89:24767
TITLE: Synthesis and characterization of phenylthiohydantoin derivatives of amino-acids protected in their side-chain functions, and their application for monitoring solid-phase peptide synthesis
AUTHOR(S): Raulais, Daniel J. P.; Rivaille, Pierre C.; Daguilhanes, Bruno; Lefevre, Gerard J. G.; Milhaud, Gerard
CORPORATE SOURCE: CNRS, Paris, Fr.
SOURCE: J. Chem. Res. (S) (1978), (1), 11
CODEN: JRPSDC
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Phenylthiohydrantoin derivs. of 11 amino acids protected in their side-chain functions, which could be obtained during the sequential degrdn. of a synthetic peptide bound to a solid support, were prepd. and analyzed by assocg. gas liq. chromatog. and thin layer chromatog. The phenylthiohydantoin derivs. of 19 unprotected amino acids are also reported. This monitoring procedure was used to check the degree of completion of difficult steps during the prepn. of the 1-34 active fragment of human parathormone and to control the purity of [8-norvaline] human calcitonin.
IT **29635-99-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, for monitoring solid-phase peptide synthesis)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



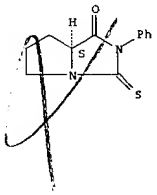
L12 ANSWER 172 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1978:185497 CAPLUS
DOCUMENT NUMBER: 88:185497
TITLE: Protein microsequencing using high-pressure liquid chromatography of phenylthiohydantoin amino acids
AUTHOR(S): Margolies, Michael N.; Brauer, Andrew
CORPORATE SOURCE: Dep. Surg., Massachusetts Gen. Hosp., Boston, Mass., USA
SOURCE: J. Chromatogr. (1978), 148(2), 429-39
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Phenylthiohydantoin (PTH)-amino acid derivs. were sepd. and quantitated by using gradient elutions with AcCN on columns of Microbondapak C18. The low signal-to-noise ratio and high sensitivity of the detection system permit quantitation of .gtoreq.10 pmol PTH-amino acids from the sequencer. This high sensitivity was used advantageously in conjunction with a 0.1M Quadrol sequencer program; the sequence of 2.7 nmol myoglobin was obtained for 32 successive cycles of Edman degrdn. with high-pressure liq. chromatog. as the sole method of identification of the PTH-amino acids. All of the PTH-amino acids were detected at 254 nm; the detection of PTH-threonine as PTH-dehydrothreonine was enhanced by detection at 313 nm.
IT **4333-21-5**
RL: ANST (Analytical study)
(sepn. and detn. of, by high-pressure liq. chromatog.)
RN 4333-21-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo- (9CI) (CA INDEX NAME)



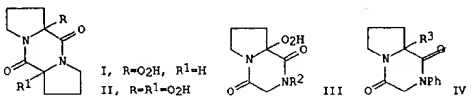
L12 ANSWER 173 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1978:148364 CAPLUS
DOCUMENT NUMBER: 88:148364
TITLE: Methanol solvent system for rapid analysis of phenylthiohydantoin amino acids by high-pressure liquid chromatography
AUTHOR(S): Bhown, Ajit S.; Mole, John E.; Weissinger, Arthur; Bennett, J. Claude
CORPORATE SOURCE: Dep. Microbiol., Univ. Alabama, Birmingham, Ala., USA
SOURCE: J. Chromatogr. (1978), 148(2), 532-5
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A high-pressure liq. chromatog. method is detailed for the sepn. and detn. of amino acid-phenylthiohydantoin (PTH) derivs. in 20 min at room temp. A com. chromatograph was used that was equipped with an absorbance detector, solvent programmer, and a .mu.Bondapak C18 column (30 cm .times. 4 mm, inner diam.). Solvents used were A, H2O-MeOH-HOAc-Me2CO (900:100:2.5 mL:50 .mu.L) (pH 4.1) and B, H2O-MeOH-HOAc (100:900:0.25 mL). The column was developed with a 15-min linear gradient of 95% A + 5% B to 55% A + 45% B at 2.5 mL/min. The MeOH program in this procedure offers good reproducibility, long column life (.gtoreq.5-6 mo), room-temp. operation, and speed (20 min for sepn. of the PTH derivs.). Most derivs. have baseline sepns. Although the PTH derivs. of leucine, phenylalanine, and isoleucine in mixts. were sepd. poorly, they could be identified readily when injected sep. The PTH derivs. of valine and methionine coeluted. The amino acid profiles of a sperm whale apomyoglobin sample (20 nmol), subjected to several steps of automated Edman degrdn., are given.
IT **29635-99-2**
RL: ANST (Analytical study)
(sepn. and detn. of, chromatog.)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 173 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



L12 ANSWER 174 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1978:136967 CAPLUS
DOCUMENT NUMBER: 88:136967
TITLE: Amino acids and peptides, XXIV. Radically and photochemically initiated oxidation of amino acid derivatives
AUTHOR(S): Haeusler, Johannes; Jahn, Rudolf; Schmidt, Ulrich
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Wien, Vienna, Austria
SOURCE: Chem. Ber. (1978), 111(1), 361-6
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
GI

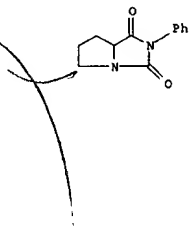


AB The photochem. oxidn. of cyclo-(Pro-Pro) in the presence of benzophenone gave 50% monohydroperoxide cis-I, 2% trans-I, 46% bishydroperoxide cis-II, and 2% trans-II, whereas the photochem. or radical oxidn. of cyclo-(DL-Pro-Sar) (Sar = MeNCH2CO) and cyclo-(DL-Pro-Gly) gave the pyrrolo[1,2-a]pyrazinediones III (R2 = Me, H, resp.). Pyrrolo[1,2-c]imidazoledione IV (R3 = H) was radically oxidized to IV (R3 = O2H).

IT 2221-09-2
RL: RCT (Reactant)
(radical oxidn. of)

RN 2221-09-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-phenyl- (9CI) (CA INDEX NAME)

L12 ANSWER 174 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



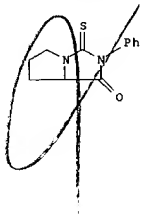
L12 ANSWER 175 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1978:117175 CAPLUS
DOCUMENT NUMBER: 88:117175
TITLE: The use of methanol in high-performance liquid chromatography of phenylthiohydantoin-amino acids
AUTHOR(S): Zeeuws, R.; Strosberg, A. D.
CORPORATE SOURCE: Lab. Chem. Proteinen, Vrije Univ. Brussel, Sint-Genesius-Rode, Belg.
SOURCE: FEBS Lett. (1978), 85(1), 68-72
CODEN: FEBLAL; ISSN: 0014-5793
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A fast, inexpensive, safe, and simple high-performance liq. chromatog. (HPLC) method was developed for the identification of amino acid-phenylthiohydantoin (PTH) derivs. for use in automated Edman degrdn. procedures. A com. chromatograph was used with a solvent programmer for gradient elution and a Microbondapak C18 (10 .mu.m) column (3.9 mm .times. 30 cm). The buffers used were: A, 23% MeOH in 0.005M NaOAc (pH 5.3)-20 .mu.L Me2CO; B, 44% MeOH; and C, 22% MeOH-5% HOAc. In program 1, for sepn. of org.-phase sol. derivs., a gradient was generated by using curve 10 of a Waters Model 660 programmer for 3 min with solvent B, followed by isocratic elution for 13 min. Program 2, for the sepn. of aq. phase-PTH derivs. of arginine, histidine, and cystine, was an isocratic elution with solvent C. In 16 min, 17 PTH derivs. could be sepd. under the given conditions. All org. phase-sol. PTH derivs., except the valine/methionine pair, which can be distinguished by gas or thin-layer chromatog., were identified easily. Although the isoleucine and phenylalanine derivs. were not well resolved, they could be distinguished by their retention times. The lysine and leucine derivs. were resolved completely by slight changes in temp. or MeOH concn. Tryptophan-PTH was sepd. completely from the other apolar PTH derivs. The method is illustrated by the anal. of samples obtained from the automated Edman degrdn. of Lotus tetragonolobus lectin.

IT 4333-21-5
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, by high-performance liq. chromatog., methanol in)

RN 4333-21-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo- (9CI) (CA INDEX NAME)

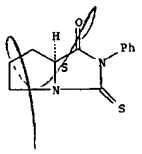
L12 ANSWER 175 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



L12 ANSWER 176 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1978:2537 CAPLUS
DOCUMENT NUMBER: 88:2537
TITLE: High-pressure liquid chromatography of amino acids and dipeptides on a tripeptide bonded stationary phase
AUTHOR(S): Fong, Godwin Wing-Kin; Grushka, Eli
CORPORATE SOURCE: Dep. Chem., State Univ. New York, Buffalo, N. Y., USA
SOURCE: J. Chromatogr. (1977), 142, 299-309
CODEN: JOCRAM
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A bonded tripeptide (L-valyl-L-phenylalanyl-L-valine) phase was used as a stationary phase in liq. chromatog. Unique retention orders and retention variations are shown for phenylthiohydantoin (PTH) derivs. of amino acids and isomeric dipeptides by using acidic and basic mobile phases. The 25 PTH-amino acids studied have different capacity ratios when 1% citric acid in water (.apprx.2.5 pH) is used as the mobile phase. The anal. time for these amino acid derivs. could be shortened without a loss in the resoln. by adding 5% MeOH to the above mobile phase. Of particular importance is the fact that the basic amino acids are eluted first. Isomeric dipeptides were resolved by using deionized water (pH 5.5) and 1% Na citrate in water (pH 7.9) as mobile phases. The nature of the mobile phases, the pH, and the ionic strength are the important factors affecting the selectivity and efficiency of the sepns. of amino acids and dipeptides.
IT **29635-99-2**
RL: ANT (Analyte); ANST (Analytical study)
(chromatog. of, high-pressure liq., on tripeptide bonded stationary phase)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

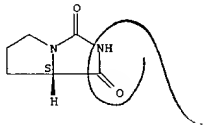
Absolute stereochemistry.

L12 ANSWER 176 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

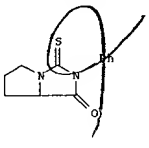


L12 ANSWER 177 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1977:567412 CAPLUS
DOCUMENT NUMBER: 87:167412
TITLE: A circular dichroism and nuclear magnetic resonance study of hydantoins and 3-phenyl-2-thiohydantoins
AUTHOR(S): Poupaert, Jacques H.; Claesen, Michel; Degelaen, Jacques; Dumont, Pierre; Toppet, Suzanne
CORPORATE SOURCE: Sch. Pharm., Univ. Louvain, Brussels, Belg.
SOURCE: Bull. Soc. Chim. Belg. (1977), 86(6), 465-72
CODEN: BSCBAG
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The CD of hydantoins and 3-phenyl-2-thiohydantoins related to the same .alpha.-amino acid were used to establish empirical rules for the assignment of abs. configuration. A relation was obtained between the (S)-configuration and a neg. Cotton effect for the 5-alkyl series and pos. Cotton effect for the 5-aryl series at 230-40 nm. The reversal in the Cotton effect was due to the homoconjugation of the Ph group and the C-4 oxo group. Mol. rotation shifts calcd. by the Freudenberg rule agreed with the exptl. data. The 1H and 13C NMR of the hydantoins and thiohydantoins were discussed.
IT **40856-87-9**
RL: PRP (Properties)
(CD of, abs. configuration in relation to)
RN 40856-87-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-, (7aS)- (9CI) (CA INDEX NAME)

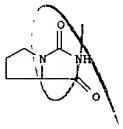
Absolute stereochemistry.



L12 ANSWER 178 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1977:117067 CAPLUS
DOCUMENT NUMBER: 86:117067
TITLE: Mass spectrometric identification of amino acid phenylthiohydantoins in the automatic sequencing of proteins
AUTHOR(S): Nazimov, I. V.; Levina, N. B.; Bogdanova, I. A.; Rosynov, B. V.
CORPORATE SOURCE: M. M. Shemyakin Inst. Bioorg. Chem., Moscow, USSR
SOURCE: Bioorg. Khim. (1977), 3(2), 192-9
CODEN: BIKHD7
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Electron impact mass spectrometry (MS) was used for the anal. of 3-phenyl-2-thiohydantoin (PTH) derivs. of amino acids produced during automatic anal. of polypeptides. Emphasis was placed on MS detn. of serine, threonine, cysteine, glutamine, asparagine, tryptophan, lysine, and histidine. Optimal conditions for mass spectral anal. were found, and the sensitivity limits of the method were evaluated. Reliable identification generally could be done by using 3 nmol PTH. MS was used for detn. of the primary structure of leghemoglobin II from yellow lupin (Lupinus luteus) root nodules.
IT **4333-21-5**
RL: PRP (Properties)
(mass spectrum of)
RN 4333-21-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo- (9CI) (CA INDEX NAME)

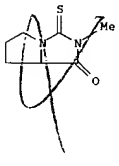


L12 ANSWER 179 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1977:115687 CAPLUS
DOCUMENT NUMBER: 86:115687
TITLE: Smoke composition. An extensive investigation of the water-soluble portion of cigarette smoke
AUTHOR(S): Schumacher, Joseph N.; Green, Charles R.; Best, Freddie W.; Newell, Marjorie P.
CORPORATE SOURCE: Res. Dep., R. J. Reynolds Tob. Co., Winston-Salem, N. C., USA
SOURCE: J. Agric. Food Chem. (1977), 25(2), 310-20
CODEN: JAFCAU
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Smoke condensate from 70 mm nonfiltered cigarettes smoked under std. conditions was collected in dry ice cooled traps and partitioned between ether and water. The water-sol. portion (.apprx.38%) was chromatographed with gradient solvent systems on silicic acid to give 9 fractions. Further sepn. of these fractions by gas chromatog. permitted isolation of 479 components. Identifications of most of these components were based on IR, mass, and NMR spectra, and gas chromatog. retention times, and comparison of these data with those of authentic samples. Of the 479 isolates identified, 387 are reported for the first time as tobacco smoke components; these include 19 acids, 61 lactones, 32 esters, 41 amides, 21 imides, 45 aldehydes and ketones, 45 alcs., 30 pyridine derivs., 25 imidazoles, 31 lactams, 23 miscellaneous nitrogen heterocyclic compds., and 14 miscellaneous compds.
IT **5768-79-6**
RL: BIOL (Biological study)
(of tobacco smoke condensate)
RN 5768-79-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro- (9CI) (CA INDEX NAME)



L12 ANSWER 179 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

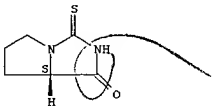
L12 ANSWER 180 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1977:1005 CAPLUS
DOCUMENT NUMBER: 86:1005
TITLE: High-protein radiomutant form of spring barley
AUTHOR(S): Volodin, V. G.; Zaben'kova, K. I.; Lisovskaya, Z. I.; Kipnas, E. A.; Kartel, N. A.
CORPORATE SOURCE: USSR
SOURCE: Issled. Teor. Prikl. Genet. (1975), 95-101.
Editor(s): Rokitskii, P. F.; Khotyleva, L. V. "Nauka i Tekhnika": Minsk, USSR.
CODEN: 34FCAY
DOCUMENT TYPE: Conference
LANGUAGE: Russian
AB A high-protein mutant of spring barley was obtained by irradiating Erectum 106 with 20 kR. The protein contents (in g/1000 grains) of the original strain, the mutant, and the std. (Moskovskij 121) were 6.01, 7.12, and 4.78, resp. The amino acid content was also elevated in the mutant, and the improved quality of this mutant barley permitted its utilization despite a lower yield.
IT **22712-58-9**
RL: BIOL (Biological study)
(of barley, plant breeding in relation to)
RN 22712-58-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo- (9CI) (CA INDEX NAME)



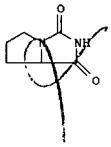
=> d ibib abs hitstr 181-208

L12 ANSWER 181 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1976:577924 CAPLUS
DOCUMENT NUMBER: 85:177924
TITLE: Mass spectrometric identification of amino acid thiohydantoins
AUTHOR(S): Suzuki, Tateo; Song, Kyung-Duck; Itagaki, Yasuhiro; Tuzimura, Katura
CORPORATE SOURCE: Fac. Agric., Tohoku Univ., Sendai, Japan
SOURCE: Org. Mass Spectrom. (1976), 11(6), 557-68
CODEN: ORMSBG
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Amino acid thiohydantoins were identified by electron impact and chem. ionization mass spectrometry. The thiohydantoin method is useful for stepwise peptide sequencing from the carboxyl terminus; the sequence of a model tripeptide was detd. as an example. The method does not work for peptides contg. proline as the C-terminal unit as cleavage of the peptide bond is not achieved.
IT **61160-12-1**
RL: PRP (Properties)
(mass spectrum of)
RN 61160-12-1 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-3-thioxo-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

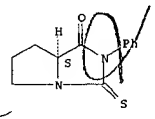


L12 ANSWER 182 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1976:150948 CAPLUS
DOCUMENT NUMBER: 84:150948
TITLE: Mass spectra of amino acid hydantoins
AUTHOR(S): Suzuki, Tateo; Tuzimura, Katura
CORPORATE SOURCE: Fac. Agric., Tohoku Univ., Sendai, Japan
SOURCE: Agric. Biol. Chem. (1976), 40(1), 225-6
CODEN: ABCHA6
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Mass spectra of amino acid hydantoins, prepd. from the amino acid and KCN, were studied. Mol. peaks appeared with small intensity or not at all as their volatility was lower than that of the thiohydantoin analogs and the hydantoins with polar functional side groups did not give mol. ions.
IT **5768-79-6**
RL: PRP (Properties)
(mass spectra of)
RN 5768-79-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro- (9CI) (CA INDEX NAME)

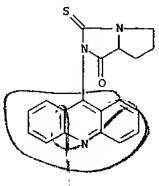


L12 ANSWER 183 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1976:56100 CAPLUS
DOCUMENT NUMBER: 84:56100
TITLE: Nuclear magnetic resonance studies of phenylthiohydantoin amino acids
AUTHOR(S): Tsai, C. S.; Fraser, N. L.; Avdovich, H.; Farant, J. P.
CORPORATE SOURCE: Dep. Chem., Carleton Univ., Ottawa, Ont., Can.
SOURCE: Can. J. Biochem. (1975), 53(9), 1005-9
CODEN: CJBIAE
DOCUMENT TYPE: Journal
LANGUAGE: English
AB PMR spectra of 3-phenyl-2-thiohydantoin derivs. of common amino acids in Me2SO-2H6 were recorded. Spectral data pertaining to characteristic protons for diagnostic purpose were compiled. Their application to the N-terminal amino acid anal. of peptide by Edman degrdn. was examd.
IT **29635-99-2**
RL: PRP (Properties)
(NMR of)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 184 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1975:563972 CAPLUS
DOCUMENT NUMBER: 83:163972
TITLE: Polycyclic aromatic isothiocyanate compounds as fluorescent labeling reagents
AUTHOR(S): Sinsheimer, J. E.; Jagodic, V.; Polak, Lj.; Hong, D. D.; Burckhalter, J. H.
CORPORATE SOURCE: Coll. Pharm., Univ. Michigan, Ann Arbor, Mich., USA
SOURCE: J. Pharm. Sci. (1975), 64(6), 925-30
CODEN: JPMSAE
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Polycyclic isothiocyanates and their derivs. I [R = NCS, H, NHCSNHR2 (R2 = CH2Ph, CH2CO2H, R1 = H, NCS, Me], II (R = NCS, NHCSNHBu), III (R = NCS, NHCSNHCH2Ph, and IV [R = NHCSNHR4 (R4 = Bu, Ph, CH2CO2H, NHCSNEt2, NHCSOEt, NHCSNHCH2CH2NEt2, CH2C6H4R4-4 (R4 = NH2, NCS), NHCH2CH2C6H4NCS-4, etc.; R1 = H, MeO, NCS, NHCSNHCH2Ph; R2 = H, Cl] were prepd. and evaluated as potential protein labeling reagents and in fluorescent microanalysis of amines. 9-Acridine derivs. were the most promising.
IT **57002-51-4P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and fluorescence of)
RN 57002-51-4 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, 2-(9-acridinyl)hexahydro-3-thioxo- (9CI)
(CA INDEX NAME)



L12 ANSWER 185 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1975:524029 CAPLUS
DOCUMENT NUMBER: 83:124029
TITLE: Light-sensitive material for color photography
INVENTOR(S): Arai, Atsuaki; Oishi, Yasushi
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd.
SOURCE: Ger. Offen., 72 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2429637	A1	19750116	DE 1974-2429637	19740620
JP 50019435	A2	19750228	JP 1973-69383	19730620
US 3891445	A	19750624	US 1974-480456	19740618
FR 2234589	A1	19750117	FR 1974-21405	19740620
BR 7405061	A0	19750121	BR 1974-5061	19740620
GB 1439106	A	19760609	GB 1974-27508	19740620

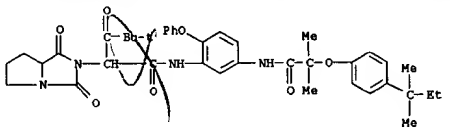
PRIORITY APPLN. INFO.: JP 1973-69383 19730620

AB Color formers with an oleophilic, diffusion-resistant phenoxyisobutyramido group contg. a total of 18-32 C atoms require only a small amt. of a solvent (b. >75.degree.) for their dispersion in Ag halide emulsions and yield dyes resistant to heat and moisture. Furthermore they are readily purified, do not crystallize, dissolve or diffuse in the developer. For their prepn. a cyan, magenta, or yellow color former contg. an NH2 group is reacted with a phenoxyisobutyryl chloride, such as ClCOC(Me)2O-m-C6H4C15H31. Thus, .alpha.-pivaloyl-2-chloro-5-[.alpha.-(3-pentadecylphenoxy)isobutyramido]acetanilide 3 g was dissolved at 60.degree. in a mixt. of di-Bu phthalate 1.5, EtOAc 2 ml, and Na bis(2-ethylhexyl) .alpha.-sulfosuccinate 150 mg, dispersed in 25 ml of an aq. soln. of gelatin 2 g at 50.degree., and added to a Ag(Br,I) emulsion.

IT **56534-47-5**
RL: TEM (Technical or engineered material use); USES (Uses)
(photog. coupler)

RN 56534-47-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-2(3H)-acetamide, .alpha.-(2,2-dimethyl-1-oxopropyl)-N-[5-[[2-[4-(1,1-dimethylpropyl)phenoxy]-2-methyl-1-oxopropyl]amino]-2-phenoxyphenyl]tetrahydro-1,3-dioxo- (9CI) (CA INDEX NAME)

L12 ANSWER 185 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



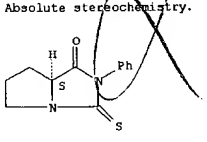
L12 ANSWER 186 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1975:497878 CAPLUS
DOCUMENT NUMBER: 83:97878
TITLE: Oscillopolarographic examination of standard PTH (phenylthiothiohydantoin) amino acids
AUTHOR(S): Iskierko, Jerzy; Bilinski, Stanislaw; Gospodarek, Jerzy; Gorski, Andrzej
CORPORATE SOURCE: Inst. Chem. Podstawowych, Akad. Med. Lublinie, Lublin, Pol.
SOURCE: Ann. Univ. Mariae Curie-Sklodowska, Sect. D (1974), 29, 135-41
CODEN: AUMKAS
DOCUMENT TYPE: Journal
LANGUAGE: Polish

AB Oscillopolarog. activity of 21 PTH amino acids was detd. in 3 basic electrolytes. The PTH amino acids showed activity in at least 1 basic electrolyte. The Q values of cathodic and anodic indentations permitted differentiation and identification of the PTH amino acids. The identification can be used to det. the amino acid sequence of proteins and peptides by Edman's method.

IT **29635-99-2**
RL: PROC (Process)
(oscillopolarog. identification of)

RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

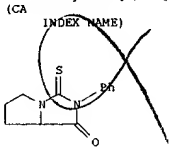


L12 ANSWER 187 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1974:474294 CAPLUS
DOCUMENT NUMBER: 81:74294
TITLE: X-ray diffraction studies of phenylthiohydantoins of amino acids
AUTHOR(S): Guha, A.; Das Gupta, Shampa
CORPORATE SOURCE: Dep. Chem., Kalyani Univ., Kalyani, India
SOURCE: Indian J. Biochem. Biophys. (1973), 10(4), 299-300
CODEN: IJBBBQ
DOCUMENT TYPE: Journal
LANGUAGE: English

AB By the use of x-ray diffraction, the intermol. spacings (d-values) of phenylthiohydantoins of some amino acids were obtained. The results may be useful in characterizing the amino acids in the Edman method of sequence studies.

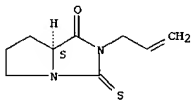
IT **4333-21-5**
RL: PROC (Process)
(x-ray diffraction of)

RN 4333-21-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo- (9CI) (CA INDEX NAME)



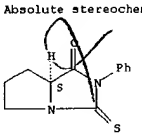
L12 ANSWER 188 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1974:142755 CAPLUS
DOCUMENT NUMBER: 80:142755
TITLE: Allyl isothiocyanate in the synthesis of 3-allyl-2-thiohydantoins from amino acids and in the degradation of proteins
AUTHOR(S): Nowak, Kornel
CORPORATE SOURCE: Inst. Biochem. Biophys., Sch. Med., Wroclaw, Pol.
SOURCE: Rocz. Chem. (1973), 47(12), 2377-8
CODEN: ROCHAC
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A series of 3-allyl-2-thiohydantoins were prepd. in 45-98% yield from CH2CHCH2NCS (I) and alanine, glycine, isoleucine, leucine, aspartic acid, tryptophan, valine, phenylalanine, tyrosine, and proline. In order to assess the usefulness of I in detg. the sequence of amino acids in protein structures, the reagent was used with pos. results for degradative sequential anal. of N-terminal amino acids in the A and B chains of insulin.
IT **52065-51-7P**
RL: PREP (Preparation)
(prepn. of, amino acid sequence detn. in proteins in relation to)
RN 52065-51-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-(2-propenyl)-3-thioxo-, (S)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 189 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1974:83586 CAPLUS
DOCUMENT NUMBER: 80:83586
TITLE: Hydrolysis of phenylthiohydantoin amino acids
AUTHOR(S): Klimek, Janusz; Wronska, Jolanta
CORPORATE SOURCE: Inst. Chem. Podstawowych, Akad. Med., Lublin, Pol.
SOURCE: Ann. Univ. Mariae Curie-Sklodowska, Sect. D (1972), 27, 197-202
CODEN: AUMKAS
DOCUMENT TYPE: Journal
LANGUAGE: Polish
AB The 16 phenylthiohydantoin (PTH) amino acids were hydrolyzed with 5.7 NHCl at 135-150.degree. for 16 hr or with satd. aq Ba(OH)2 at 105-135.degree. for 16 hrs. The free amino acid obtained depended on the nature of PTH-amino acid and the technique of hydrolysis and varied from 3.7 to 85% as detd. by paper chromatog.
IT **29635-99-2**
RL: RCT (Reactant)
(hydrolysis of)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-
(9CI) (CA INDEX NAME)

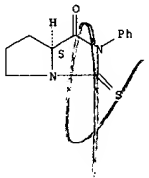
Absolute stereochemistry.



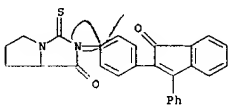
L12 ANSWER 190 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1974:71070 CAPLUS
DOCUMENT NUMBER: 80:71070
TITLE: Identification of PTH [phenylhydantoin] amino acids by high-performance liquid chromatography
AUTHOR(S): Frank, G.; Strubert, W.
CORPORATE SOURCE: Inst. Molekularbiol. Biophys., Eidg. Tech. Hochsch., Zurich-Hoenggerberg, Ger.
SOURCE: Chromatographia (1973), 6(12), 522-4
CODEN: CHRGB7
DOCUMENT TYPE: Journal
LANGUAGE: German
AB Sixteen PTH amino acids were sepd. in two liq. chromatog. systems, one of which separates 9 hydrophobic, the other 7 hydrophilic compds. The running time for each chromatogram is only 7 mins. and all the components were evaluated quant. in amts. down to 1 nanomole or less. Sepn. of PTH amino acids by high performance liq. chromatog. appears to be superior to thin-layer chromatog. and gas chromatog.
IT **31364-82-6**
RL: ANT (Analyte); ANST (Analytical study)
(chromatog. of)
RN 31364-82-6 CAPLUS

L12 ANSWER 191 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1974:37435 CAPLUS
DOCUMENT NUMBER: 80:37435
TITLE: Acetylation of phenylthiohydantoins of amino acids
AUTHOR(S): Inglis, A. S.; Nicholls, P. W.
CORPORATE SOURCE: Div. Protein Chem., CSIRO, Parkville, Aust.
SOURCE: J. Chromatogr. (1973), 86(1), 117-22
CODEN: JOCRAM
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Acetylation of amino acid phenylthiohydantoins was studied and the chromatog. behavior of the derivs. compared with the phenylthiohydantoins. Some acetylated derivs. were better suited than the parent phenylthiohydantoins to gas chromatog. anal.
IT **29635-99-2**
RL: ANT (Analyte); ANST (Analytical study)
(gas chromatog. of)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

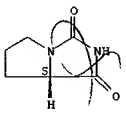


L12 ANSWER 192 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1973:401613 CAPLUS
DOCUMENT NUMBER: 79:1613
TITLE: Interaction of 2-p-isothiocyanophenyl-3-phenylindone with peptides and proteins
AUTHOR(S): Ivanov, Chavdar P.; Mancheva, Ivanka N.
CORPORATE SOURCE: Dep. Org. Chem., Higher Inst. Chem. Technol., Sofia, Bulg.
SOURCE: Anal. Biochem. (1973), 53(2), 420-30
CODEN: ANBCA2
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The conditions of interaction with peptide chains of a new reagent for detn. of amino acid sequence, (2-p-isothiocyanophenyl-3-phenylindone) were established. The conditions for cleavage of the N-terminal amino acid as a colored diphenylindonyl-substituted thiohydantoin deriv. were found as well. The .lambda.max and .epsilon.max of diphenylindonyl thiohydantoin derivs. of all common amino acids usually found in proteins were detd. The .epsilon.max values were .apprx. 3 times higher than the corresponding values of phenylthiohydantoin derivs.
IT **42353-03-7**
RL: PRP (Properties)
(uv spectrum of)
RN 42353-03-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-[4-(1-oxo-3-phenyl-1H-inden-2-yl)phenyl]-3-thioxo- (9CI) (CA INDEX NAME)



L12 ANSWER 193 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1973:148205 CAPLUS
DOCUMENT NUMBER: 78:148205
TITLE: Optical rotatory dispersion and circular dichroism of amino acid hydantoins
AUTHOR(S): Suzuki, Tateo; Igarashi, Keiji; Hase, Kieko; Tuzimura, Katura
CORPORATE SOURCE: Fac. Agric., Tohoku Univ., Sendai, Japan
SOURCE: Agr. Biol. Chem. (1973), 37(2), 411-16
CODEN: ABCHA6
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Hydantoins were prepd. from 17 amino acids and KOCN. The hydantoins of 13 of the amino acids showed neg. Cotton effects at 238-245 nm. That of tyrosine was at 248 nm and that of tryptophan at 256 nm. Proline hydantoin showed a neg. Cotton effects at 233 nm, a cross-over point at 245 nm and a peak at .apprx.254 nm. According to the octant rule the neg. Cotton effects were assigned to the C-4 CO groups of the hydantoins.
IT **40856-87-9P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and Cotton effect of)
RN 40856-87-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-, (7aS)- (9CI) (CA INDEX NAME)

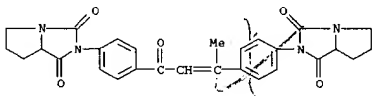
Absolute stereochemistry.



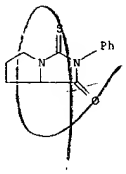
L12 ANSWER 194 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1973:147963 CAPLUS
DOCUMENT NUMBER: 78:147963
TITLE: Chalcone derivatives
INVENTOR(S): Oshiro, Susumu; Nagura, Takeo; Sugihara, Yukio; Okamoto, Koji; Ishida, Ryuichi; Shintomi, Keiichi
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd.
SOURCE: Japan. Kokai, 3 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 48019594	B4	19730312	JP 1971-55100	19710722

GI For diagram(s), see printed CA Issue.
AB The title compds. (I), antispasmodics and tranquilizers, were prepd. by treating 4,4'-diprolylaminochalcones with HCHO or with N,N'-carbonyldiimidazole (carbonalating agent). E.g., 18.5 g 4,4'-bis(L-prolylamino)-.beta.-methylchalcone in MeOH was stirred 5 hr at 50.degree. with 13.4 g 37% HCHO to give 97% I (X = CH2, R1 = Me, R2 = R3 = H). Similarly prepd. were the following I (X, R1, R2, R3, and % yield given): CH2, H, Me, H, 85; CH2, H, H, H, 72% (dihydrochloride); CH2, H, H, Me, 82 (dihydrochloride); CO, Me, H, H, 45.
IT **41038-72-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 41038-72-6 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazole-1,3(2H)-dione, tetrahydro-2-[4-[1-methyl-3-oxo-3-[4-(tetrahydro-1,3-dioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)phenyl]-1-propenyl]phenyl]- (9CI) (CA INDEX NAME)



L12 ANSWER 195 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1972:82428 CAPLUS
DOCUMENT NUMBER: 76:82428
TITLE: Acid hydrolysis of phenylthiohydantoins of amino acids
AUTHOR(S): Inglis, A. S.; Nicholls, P. W.; Roxburgh, C. M.
CORPORATE SOURCE: Div. Protein Chem., CSIRO, Parkville, Aust.
SOURCE: Aust. J. Biol. Sci. (1971), 24(6), 1247-50
CODEN: AJBSAM
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Hydrolysis of phenylthiohydantoins with refluxing HI for 24 hr gave good yields of recognizable products except for methionine. The thiohydantoins of threonine, serine, and tryptophan were converted to .alpha.-aminobutyric acid, alanine, and a mixt. of glycine and alanine resp. If the thiohydantoin of methionine was oxidized prior to hydrolysis, a good yield of methionine sulfone was obtained.
IT **4333-21-5**
RL: RCT (Reactant)
(hydrolysis of, acid)
RN 4333-21-5 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo- (9CI) (CA INDEX NAME)

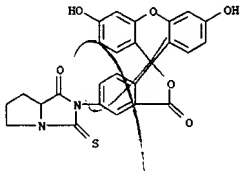


L12 ANSWER 196 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1971:420961 CAPLUS
DOCUMENT NUMBER: 75:20961
TITLE: Reaction of fluorescein-isothiocyanate with proteins and amino acids. III. Syntheses of trifluoroacetic acid salts of fluorescein-thiohydantoin amino acids and their spectrometric studies
AUTHOR(S): Kawauchi, Hiroshi; Tuzimura, Katura
CORPORATE SOURCE: Fac. Agric., Tohoku Univ., Sendai, Japan
SOURCE: Agr. Biol. Chem. (1971), 35(2), 150-7
CODEN: ABCHA6
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The ir spectrum of nitrofluorescein equilibrated with 6N HCl showed that nitrofluorescein-HCl (I, R = NO2, X = Cl) decompd. with water to give II reversibly. Fluorescein and its derivs. readily formed salts I (X = F3CCO2) with F3CCO2H. Fluorescein isothiocyanate was treated with L-amino acids, glycine, alanine, valine, leucine, isoleucine, proline, hydroxyproline, aspartic acid, glutamic acid, phenylalanine, tyrosine, methionine, S-carboxymethylcysteine, arginine, histidine, and dehydrothreonine, and cyclized (HCl) to give the corresponding thiohydantoin derivs. (III) or IV, which were converted into F3CCO2H salts whose spectral data (uv, visible, fluorescent, ORD, ir, NMR) were given. The F3CCO2H salts of III and IV were superior to III and IV as std. materials for N-terminal anal.
IT **32636-46-7P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and spectra of)
RN 32636-46-7 CAPLUS
CN Fluorescein, 5-(1-thio-1,2-pyrrolidinedicarboximido)-, mono(trifluoroacetate) (salt) (8CI) (CA INDEX NAME)

CM 1

CRN 47758-46-3
CMF C26 H18 N2 O6 S

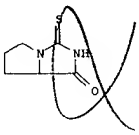
L12 ANSWER 196 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



CM 2

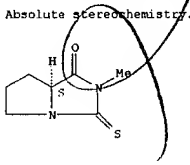
CRN 76-05-1
CMF C2 H F3 O2

L12 ANSWER 197 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1971:406263 CAPLUS
DOCUMENT NUMBER: 75:6263
TITLE: Formation of thiohydantoin derivative of proline from C-terminal of peptides
AUTHOR(S): Kubo, Hiroaki; Nakajima, Terumi; Tamura, Zenzo
CORPORATE SOURCE: Fac. Pharm. Sci., Univ. Tokyo, Tokyo, Japan
SOURCE: Chem. Pharm. Bull. (1971), 19(1), 210-11
CODEN: CPBTAL
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 1-Acetyl-2-thiohydantoins were quant. prepd. by treatment of acetylated amino acids in F3CCO2H and AcCl with HSCN in dioxane: among 13 acetylated amino acids, acetylproline gave deacetylated hydantoin. Z-Glycylproline gave both prolylthiohydantoin and Z-glycylthiohydantoin. Z = benzyloxycarbonyl.
IT **32085-78-2P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, from C-terminal proline of peptides)
RN 32085-78-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-3-thioxo- (9CI) (CA INDEX NAME)

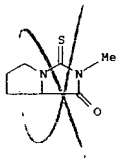


L12 ANSWER 198 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1971:60936 CAPLUS
DOCUMENT NUMBER: 74:60936
TITLE: Optical rotatory properties of methylisothiocyanate-amino acid adducts
AUTHOR(S): Toniolo, Claudio
CORPORATE SOURCE: Ist. Chim. Org., Univ. Padova, Padua, Italy
SOURCE: Tetrahedron (1970), 26(23), 5479-88
CODEN: TETRAB
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Definite information concerning the optical configurations of amino acids in peptides has been obtained from an investigation of the CD of their adducts with methyl isothiocyanate.
IT **28868-23-7**
RL: PRP (Properties)
(circular dichroism of)
RN 28868-23-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo-, (7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 199 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1971:54160 CAPLUS
DOCUMENT NUMBER: 74:54160
TITLE: Gas chromatographic identification of the thiohydantoins of degradation products peptides and proteins
AUTHOR(S): Tschesche, Harald; Obermeier, Rainer; Kupfer, Sigrid
CORPORATE SOURCE: Lab. Org. Chem. Biochem., Tech. Univ. Muenchen, Munich, Ger.
SOURCE: Angew. Chem., Int. Ed. Engl. (1970), 9(11), 893-4
CODEN: ACIEAY
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Naturally occurring amino acids can be chromatographed as their 3-methyl-2-thiohydantoin derivs. (I). The acids, phenylalanine, asparagine, glutamine, tyrosine, and tryptophan, are chromatographed after treatment with MeNCS.
IT **22712-58-9**
RL: ANT (Analyte); ANST (Analytical study)
(chromatog. of, gas)
RN 22712-58-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo- (9CI) (CA INDEX NAME)

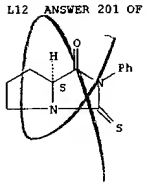


L12 ANSWER 200 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1971:40930 CAPLUS
DOCUMENT NUMBER: 74:40930
TITLE: Peripheral inhibition of thyroxine by thiohydantoins derived from amino acids
AUTHOR(S): Westerfeld, Wilfred W.; Marx, Joseph V.; Richert, Dan A.
CORPORATE SOURCE: Upstate Med. Center, State Univ. New York, Syracuse, N. Y., USA
SOURCE: J. Med. Chem. (1970), 13(6), 1179-81
CODEN: JMCMAR
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB 3-Phenyl-2-thiohydantoin (I) when substituted at the 5-position with nonpolar amino acids, such as proline and leucine, most significantly antagonized the effect of exogenous thyroxine on the induction of rat mitochondrial .alpha.-glycerophosphate dehydrogenase (EC 1.1.99.5), without affecting thyroid gland functions, whereas I substituted with polar amino acids, such as asparagine and tyrosine, was inactive. The peripheral inhibitors of thyroxine were very weak goiterogens.
IT **31364-82-6**
RL: BIOL (Biological study)
(thyroxine antagonism by)
RN 31364-82-6 CAPLUS

L12 ANSWER 201 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1970:531280 CAPLUS
DOCUMENT NUMBER: 73:131280
TITLE: Circular dichroism and configuration of .alpha.-amino acid
AUTHOR(S): Auterhoff, Harry; Hansen, J. G.
CORPORATE SOURCE: Pharm.-Chem. Inst., Univ. Tuebingen, Tuebingen, Ger.
SOURCE: Pharmazie (1970), 25(5-6), 336-40
CODEN: PHARAT
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB Seventeen optically active N-phthaloyl-.alpha.-amino acids were prepd. by condensation of phthalic anhydride with the amino acid either alone or in AcOH or dioxane or by treatment of the acid with N-carbethoxyphthalimide in an alk. medium. The Cotton effect is solvent-dependent and a correlation of the sign of the effect with configuration was impossible. Amino acid (500 mg) in 6 ml C5H5N and 6 ml H2O adjusted to pH 8.0-8.5 with 0.5N NaOH and the soln. treated with 0.6 ml PhNCS, gave the 3-phenyl-2-thiohydantoin (I), in which the asymmetric C atom is fixed in a ring so that no rotamers are expected. In 16 I CD max. (in molar ellipticity units), the signs of the Cotton effect for all derivs. of the same configuration were the same in all solvents (AcOH, MeOH, Et2O, dioxane) used; thus, pos. and neg. Cotton effects corresponded to L- and D-configurations, resp. The behavior of .alpha.-methyl-.alpha.-amino acids was investigated in the 3-phenyl-2-thiohydantoins of (-)-.alpha.-methyldopa, (+)- and (-)-isovaline, and (-)-.alpha.-methylleucine. The configuration of these derivs. was not determinable from their CD.
IT **29635-99-2**
RL: PRP (Properties)
(circular dichroism of)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)- (9CI) (CA INDEX NAME)

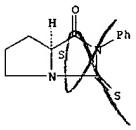
Absolute stereochemistry.

L12 ANSWER 201 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)



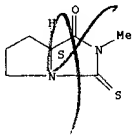
L12 ANSWER 202 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1970:506188 CAPLUS
DOCUMENT NUMBER: 73:106188
TITLE: Mass spectrometric identification of amino acid phenylthiohydantoins
AUTHOR(S): Hagenmaier, Hanspaul; Ebbighausen, W.; Nicholson, G.; Voetsch, W.
CORPORATE SOURCE: Univ. Tuebingen, Tuebingen, Ger.
SOURCE: Z. Naturforsch. B (1970), 25(7), 681-9
CODEN: ZENBAX
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB The unequivocal identification of the phenylthiohydantoin derivs. (I and II) of 21 amino acids usually occurring in proteins is possible by mass spectrometry and by combined gas chromatog.-mass spectrometry. The method is sensitive enough to be applied to the identification of phenylthiohydantoins obtained from automated Edman degradations of polypeptides. Mass spectra of I (R given) were reported: H, Me, iso-Pr, iso-Bu, sec-Bu, CH2OH, CHMeOH, CH2CO2H, CH2CONH2, CH2CH2CO2H, CH2CH2CONH2, CH2SO3H, CH2SCH2CO2H, CH2CH2SMe, (CH2)3NHC(:NH)NH2. (CH2)4NHCSNHPh, CH2Ph, CH2C6H4OH-p, 3-indolylmethyl, and 4-imidazolylmethyl. Mass spectra of II were also reported.
IT **29635-99-2**
RL: PRP (Properties)
(mass spectrum of)
RN 29635-99-2 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-phenyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

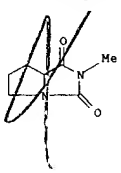


L12 ANSWER 203 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1970:488146 CAPLUS
DOCUMENT NUMBER: 73:88146
TITLE: Syntheses and gas chromatography of methylthiohydantoin-amino acids
AUTHOR(S): Okamoto, Hiroo; Okuyama, Tsuneo
CORPORATE SOURCE: Fac. Sci., Tokyo Metrop. Univ., Tokyo, Japan
SOURCE: Seikagaku (1969), 41(12), 850-9
CODEN: SEIKAQ
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
AB 3-Methyl-2-thiohydantoin derivs. of glycine, DL-alanine, L-valine, L-leucine, L-isoleucine, L-phenylalanine, DL-methionine, L-glutamate, DL-aspartate, L-glutamine, L-asparagine, L-threonine, L-serine, L-lysine, L-histidine, L-tyrosine, L-tryptophan, and L-proline were synthesized. Some of these derivs. of amino acids were separable by gas chromatography. Trimethylsilation of these derivs. enable the sepn. of all protein amino acids by gas chromatog. operated at 175-250.degree..
IT **28868-23-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 28868-23-7 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo-, (7aS)-(9CI) (CA INDEX NAME)

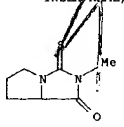
Absolute stereochemistry.



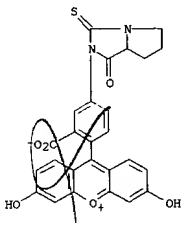
L12 ANSWER 204 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1970:477186 CAPLUS
DOCUMENT NUMBER: 73:77186
TITLE: Heterocyclizations. VII. New hydantoins with bridge-head nitrogen of spiran structure
AUTHOR(S): Capuano, Lilly; Welter, Mechthild; Zander, Rita
CORPORATE SOURCE: Inst. Org. Chem., Univ. Saarland, Saarbruecken, Ger.
SOURCE: Chem. Ber. (1970), 103(8), 2394-2402
CODEN: CHBEAM
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB Reaction of di-Me 4,5-imidazoledicarboxylate with MeNCO gave 1,3-dioxo-2-methyl-7-methoxycarbonyl-2,3-dihydro-1H- imidazo[1,5-c]imidazole (I). Similar reaction of Et prolinate or Et pipecolate gave 1,3-dioxo-2-methylperhydropyrrolo[1,2-c]imidazole (II) or -imidazo[1,5-a]pyridine (III), resp. Reaction of isatin with RNCO in EtOH-NEt3 gave Et 3-(R-substituted)-4-hydroxy-2-thiono-1,2,3,4-tetrahydro-4- quinazolinecarboxylates (IV) (where R = Me or Ph). Reaction of isatin-3-imide with RNCO gave 3-[(RNHCON:)-substituted]-1-[(RNHCO)-substituted]2-oxo-2, 3-dihydroindoles (V) (where R = Me or Ph), which on cyclization with EtOH-NEt3 gave 1',3-(R,R-disubstituted)-2,i',5h-trioxo-1,2,3, 4-tetrahydrospiro[quinazoline-4,4'-imidazolidines] (VI) (where R = Me or Ph).
IT **28567-64-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 28567-64-8 CAPLUS
CN 1,2-Pyrrolidinedicarboximide, N-methyl- (8CI) (CA INDEX NAME)



L12 ANSWER 205 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1970:133164 CAPLUS
DOCUMENT NUMBER: 72:133164
TITLE: Gas chromatography of methyl thiohydantoins of amino acids
AUTHOR(S): Attrill, James E.; Butts, William C.; Rainey, William T., Jr.; Holleman, James W.
CORPORATE SOURCE: Anal. Chem. Div., Oak Ridge Nat. Lab., Oak Ridge, Tenn., USA
SOURCE: Anal. Lett. (1970), 3(2), 59-65
CODEN: ANALBP
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The methyl thiohydantoins of 22 amino acids commonly encountered in protein sequence work were prepd. and their behavior on gas chromatog. investigated. Sixteen of these were sepd. from each other by 2 columns with different silicone stationary phases. The methyl thiohydantoins of aspartic acid, serine, arginine, carboxymethyl cysteine, and cysteic acid, which gave decompn. and a common peak in the above systems, gave unique peaks following silylation. The methyl thiohydantoin of cysteine was not successfully analyzed.
IT **22712-58-9**
RL: ANT (Analyte); ANST (Analytical study)
(gas chromatog. of)
RN 22712-58-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo- (9CI) (CA INDEX NAME)



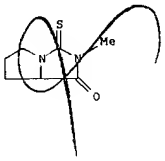
L12 ANSWER 206 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1970:44095 CAPLUS
DOCUMENT NUMBER: 72:44095
TITLE: Reaction of fluorescein-isothiocyanate with proteins and amino acids. II. Preparation of fluorescein-thiohydantoin amino acids and their thin-layer chromatography
AUTHOR(S): Kawauchi, Hiroshi; Tuzimura, Katura; Maeda, Hiroshi; Ishida, Nakao
CORPORATE SOURCE: Fac. Agr., Tohoku Univ., Sendai, Japan
SOURCE: J. Biochem. (Tokyo) (1969), 66(6), 783-9
CODEN: JOBIAO
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Amino acids react with fluorescein isothiocyanate to form fluoresceinthiocarbamoyl amino acids. Fluoresceinthiocarbamoyl amino acids were converted into fluoresceinthiohydantoin amino acids under acidic conditions. Amino acid fluoresceinthiohydantoins were successfully sepd. by thin-layer chromatog. These results are discussed in connection with their application to microanal. of amino acids, peptides, and proteins.
IT **24956-96-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 24956-96-5 CAPLUS
CN Xanthylium, 9-[2-carboxy-4-(tetrahydro-1-oxo-3-thioxo-1H-pyrrolo[1,2-c]imidazol-2(3H)-yl)phenyl]-3,6-dihydroxy-, hydroxide, inner salt (8CI)
(CA INDEX NAME)



L12 ANSWER 206 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)

L12 ANSWER 207 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1969:430677 CAPLUS
DOCUMENT NUMBER: 71:30677
TITLE: Sequential degradation of proteins and peptides
AUTHOR(S): Richards, Frank F.; Barnes, William T.; Lovins, Robert E.; Salomone, Ramon; Waterfield, Michael D.
CORPORATE SOURCE: Sch. of Med., Yale Univ., New Haven, Conn., USA
SOURCE: Nature (1969), 221(5187), 1241-4
CODEN: NATUAS
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A quant. protein degradation method using a volatile Edman reagent (MeNCS), an isotope diln. step for quantitation of the data, and an isotope ratio assay by conventional mass spectrometry is described. In this method, the peptide or protein is dissolved in 50% aq. pyridine and reacted for 1 hr. at 60.degree. with a 10 molar excess (based on available amino end groups) of MeNCS in the absence of O and light. In subsequent reactions with the 2nd NH2-terminal residue, only a 1.5 mole excess of MeNCS is required. To this aliquot is added a standardized soln. contg. a mixt. of 20 Me thiohydantoin amino-acid derivs. which are enriched in 15N and for which the exact 14N/15N ratio is known for each derivative. Excess MeNCS is removed during 2 hrs. in vacuo at 6.degree.. The residue is treated with CF3CO2H or CF3CF2CF2CO2H for 10 min., after which the excess acid is removed with N gas at 90.degree.. This method promotes the formation of the cyclic thiohydantoin deriv. from the N-terminal thiourea without detectable thiazolidone formation, and the product yields are >98%. Alternatively, it is possible to volatilize the thiohydantoin deriv. using hot N and a sample trap to collect the volatized deriv. Using these conditions, the method does not destroy the peptide. After removal of the excess acid, the residue is taken up in tetrahydrofuran, and a nonquant. aliquot contg. 1-10 mg. thiohydantoins is transferred to a small capillary. The solvent is removed under vacuum, and the capillary is heated slowly in a mass spectrometer. This method permits partial sepn., in order of volatility, making it easier to identify and det. the amts. of each Me thiohydantoin in the mixt. The mass spectra are further simplified by using a low ionizing voltage (10 ev.) which produces spectra contg. primarily the mol. ions and only a few of the more abundant fragment ions. Clearly identifiable mol. ions are observed for all

L12 ANSWER 207 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
derivs. except S-aminoethylcysteine (which may be identified by a fragment ion at m/e 150). Because of ambiguities, leucine and isoleucine are identified from fragment ions at m/e 143 and m/e 102, resp. To obtain quant. information from the mass spectra, the 14N/15N ratios in the mol. ion peaks of the derivs. present in the mixt. are accurately detd. from the recorded spectrum, and any contribution from other ions is subtracted. These ratios and the initial concn. of each 15N enriched deriv. introduced permit the detn. of the exact amt. of each Me thiohydantoin formed at each N-terminal reaction. The derivs. of the common amino-acids are all sufficiently volatile to be used in this method.
IT **22712-58-9**
RL: PRP (Properties)
(mass spectrum of)
RN 22712-58-9 CAPLUS
CN 1H-Pyrrolo[1,2-c]imidazol-1-one, hexahydro-2-methyl-3-thioxo- (9CI) (CA INDEX NAME)



L12 ANSWER 208 OF 208 CAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1969:4564 CAPLUS
DOCUMENT NUMBER: 70:4564
TITLE: Preparation of diphenylindonyl-substituted thiohydantoin derivatives of some amino acids
AUTHOR(S): Ivanov, Ch. P.; Mancheva, I. N.
CORPORATE SOURCE: Inst. Chem. Technol., Sofia, Bulg.
SOURCE: Dokl. Bolg. Akad. Nauk (1968), 21(8), 785-8
CODEN: DBANAD
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Several amino acids are treated with 2-(p-isothiocyanophenyl)-3-phenylindone (I) to prep. their 3-[p-[2-(3-phenylindonyl)phenyl]]-2-thiohydantoin derivs. (II, R is the amino acid residue). To prep the II, 0.5 millimole amino acid was dissolved in 2-4 ml. 50% aq. pyridine, adjusted to pH 9 with N NaOH, heated to 40.degree., treated with 0.55 millimole I in pyridine, kept at pH 9 with N NaOH for 1 hr., dild. with an equal amt. of water, extd. several times with benzene, and treated with excess N HCl to ppt. the indonylthiocarbamyl amino acid which was sepd., extd. with AcOEt, washed with water, and evapd. to dryness in vacuo over H2SO4. N,N'-bis[p-[2-(3-phenylindonyl)phenyl]]thiourea m. 209.degree. (acetone), was obtained from the benzene exts. obtained above as a byproduct of this reaction. The crude carbamyl amino acid was dissolved in 2.5 ml. AcOH, treated slowly with 0.5 ml. 6N HCl, heated 6 hrs. at 40.degree., and cooled to cryst. the II. Addnl. II was obtained, after filtering the II from the soln., by evapg. the filtrate to dryness, washing it with water, and chromatographing it on alumina. Pure II were obtained by chromatog. on alumina with 99.75:0.25 benzene-MeOH. The chief products were eluted with this solvent mixt. dild. with an equal vol. of acetone. II prepd. were (starting amino acid, R, % yield, and m.p. given): glycine, H, 91.4, 196-8.degree.; DL-.alpha.-alanine, Me, 95.6, 233-4.degree.; DL-.alpha.-aminobutyric acid, Et, 90.0, 227-8.degree.; DL-valine, iso-Pr, 81.4, 239-40.degree.; DL-norvaline, Pr, 88.3, 261-2.degree.; L-leucine, Me2CHCH2, 95.2, 232-3.degree. (EtOH); DL-norleucine, Bu, 90.6, 207-9.degree.; DL-isoleucin, EtC(Me)H, 83.9, 221.5-2.0.degree. (EtOH); DL-phenylalanine, PhCH2, 84.6, 254-5.degree.; L-methionine, MeSCH2CH2, 94.4, 170-2.degree.; L-tyrosine, p-hydroxybenzyl,

L12 ANSWER 208 OF 208 CAPLUS COPYRIGHT 2001 ACS (Continued)
90.3, 243-4.degree.; L-glutamic acid, HO2CCH2CH2, 70, 175-7.degree. (EtOH).
IT **20806-56-8?**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 20806-56-8 CAPLUS

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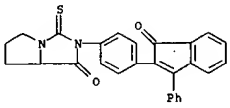
=> S 20806-56-8/RN

L13 1 20806-56-8/RN

=> D L13 SQIDE TOTAL

L13 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2001 ACS
RN 42353-03-7 REGISTRY
CN 1H-Pyrrolo[1,2-c]imidazol-1-one,
hexahydro-2-[4-(1-oxo-3-phenyl-1H-inden-2-
yl)phenyl]-3-thioxo- (9CI) (CA INDEX NAME)
FS 3D CONCORD
DR **20806-56-8**
MF C27 H20 N2 O2 S
LC STN Files: CA, CAPLUS



2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)